Methane, bromo-

Other names:

BROMOMETHANE
Bercema
Brom-O-gas
Brom-O-gaz
Brom-O-sol
Brom-methan
Bromometano
Bromure de methyle
Bromuro di metile
Broommethaan
CH3Br
CURAFUME
Celfume
Dawson 100
Detia gas ex-M
Dowfume mc-2
Dowfume mc-2 soil fumigant
Dowfume mc-33
Edco
Embafume
Fumigant-1
Halon 1001
Haltox
Iscobrome
Kayafume
MBX
METHYL BROMIDE
MeBr
Metafume
Methogas
Methybrom
Methylbromid
Metylu bromek
Monobromomethane
Pestmaster
Profume
R 40B1
REFRIGERANT-40B1
Rcra waste number U029
Terabol

	Terr-O-gas 100
	Terr-O-gas 67
	UN 1062
	Zytox
Inchi:	InChI=1S/CH3Br/c1-2/h1H3
InchiKey:	GZUXJHMPEANEGY-UHFFFAOYSA-N
Formula:	CH3Br
SMILES:	CBr
Mol. weight [g/mol]:	94.94
CAS:	74-83-9

Physical Properties

Property code	Value	Unit	Source
affp	664.20	kJ/mol	NIST Webbook
aigt	810.37	K	KDB
basg	638.00	kJ/mol	NIST Webbook
dm	1.80	debye	KDB
fll	10.00	% in Air	KDB
flu	15.00	% in Air	KDB
gf	-28.18	kJ/mol	KDB
hf	-37.68	kJ/mol	KDB
hf	-34.30 ± 0.80	kJ/mol	NIST Webbook
hf	-38.00 ± 1.30	kJ/mol	NIST Webbook
hf	-37.50 ± 1.50	kJ/mol	NIST Webbook
hfl	-60.60 ± 1.30	kJ/mol	NIST Webbook
hfus	3.63	kJ/mol	Joback Method
hvap	23.00	kJ/mol	NIST Webbook
hvap	23.24	kJ/mol	NIST Webbook
ie	10.50 ± 0.20	eV	NIST Webbook
ie	10.53	eV	NIST Webbook
ie	10.53	eV	NIST Webbook
ie	10.54	eV	NIST Webbook
ie	10.54 ± 0.00	eV	NIST Webbook
ie	10.53 ± 0.02	eV	NIST Webbook
ie	10.53 ± 0.01	eV	NIST Webbook
ie	10.54 ± 0.01	eV	NIST Webbook
ie	10.53	eV	NIST Webbook
ie	10.53 ± 0.01	eV	NIST Webbook
ie	10.54	eV	NIST Webbook
ie	10.53	eV	NIST Webbook

ie	10.54	eV	NIST Webbook
ie	10.53	eV	NIST Webbook
ie	10.53 ± 0.01	eV	NIST Webbook
ie	10.70	eV	NIST Webbook
ie	10.54 ± 0.00	eV	NIST Webbook
ie	10.54	eV	NIST Webbook
ie	10.53	eV	NIST Webbook
ie	10.50 ± 0.20	eV	NIST Webbook
log10ws	-0.87		Aqueous Solubility Prediction Method
log10ws	-0.79		Estimated Solubility Method
logp	1.011		Crippen Method
mcvol	42.450	ml/mol	McGowan Method
pc	6610.00	kPa	KDB
rinpol	420.00		NIST Webbook
rinpol	415.00		NIST Webbook
rinpol	414.00		NIST Webbook
rinpol	429.00		NIST Webbook
rinpol	421.00		NIST Webbook
rinpol	429.00		NIST Webbook
rinpol	414.00		NIST Webbook
rinpol	421.00		NIST Webbook
sl	155.14	J/mol×K	NIST Webbook
tb	276.60	K	KDB
tb	277.50 ± 0.30	K	NIST Webbook
tb	276.60	K	NIST Webbook
tb	276.60	K	NIST Webbook
tb	277.65 ± 1.00	K	NIST Webbook
tc	464.00	K	KDB
tf	179.50	K	KDB
tf	179.45	K	Aqueous Solubility Prediction Method
tt	179.47 ± 0.02	K	NIST Webbook
vc	0.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	55.85	J/mol×K	473.09	Joback Method
cpg	44.65	J/mol×K	319.22	Joback Method
cpg	47.12	J/mol×K	349.99	Joback Method

cpg	49.48	J/mol×K	380.77	Joback Method
cpg	51.71	J/mol×K	411.54	Joback Method
cpg	53.83	J/mol×K	442.32	Joback Method
cpg	42.04	J/mol×K	288.44	Joback Method
cpl	78.83	J/mol×K	280.00	NIST Webbook
cpl	114.60	J/mol×K	283.00	NIST Webbook
dvisc	0.0006511	Pa×s	224.63	Joback Method
dvisc	0.0008975	Pa×s	203.37	Joback Method
dvisc	0.0013334	Pa×s	182.10	Joback Method
dvisc	0.0021998	Pa×s	160.83	Joback Method
dvisc	0.0004993	Pa×s	245.90	Joback Method
dvisc	0.0003994	Pa×s	267.17	Joback Method
dvisc	0.0003302	Pa×s	288.44	Joback Method
hfust	6.00	kJ/mol	179.50	NIST Webbook
hfust	5.98	kJ/mol	179.50	NIST Webbook
hfust	5.98	kJ/mol	179.50	NIST Webbook
hfust	0.47	kJ/mol	173.80	NIST Webbook
hvapt	25.80	kJ/mol	250.50	NIST Webbook
hvapt	23.90 ± 0.30	kJ/mol	276.66	NIST Webbook
hvapt	25.30	kJ/mol	240.50	NIST Webbook
hvapt	23.91	kJ/mol	276.60	NIST Webbook
hvapt	25.20	kJ/mol	240.00	NIST Webbook
hvapt	24.60	kJ/mol	248.50	NIST Webbook
hvapt	23.91	kJ/mol	277.50	KDB
hvapt	23.91	kJ/mol	276.71	NIST Webbook
rhol	1737.00	kg/m3	268.00	KDB
sfust	33.30	J/mol×K	179.50	NIST Webbook
sfust	2.72	J/mol×K	173.80	NIST Webbook
svapt	86.42	J/mol×K	276.71	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49022e+01
Coeff. B	-2.64173e+03
Coeff. C	-1.97200e+01
Temperature range (K), min.	179.55
Temperature range (K), max.	427.00

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.36681e+01
Coeff. B	-4.64341e+03
Coeff. C	-7.65899e+00
Coeff. D	1.03669e-05
Temperature range (K), min.	179.47
Temperature range (K), max.	467.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74839&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1529
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1529
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535

Legend

affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions

hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume