Methane, dibromodichloro-

Other names:	Dibromodichloromethane
	CCl2Br2
	Carbon dibromide dichloride
Inchi:	InChI=1S/CBr2Cl2/c2-1(3,4)5
InchiKey:	IHUREIPXVFKEDT-UHFFFAOYSA-N
Formula:	CBr2Cl2
SMILES:	ClC(Cl)(Br)Br
Mol. weight [g/mol]:	242.72
CAS:	594-18-3

Physical Properties

Property code	Value	Unit	Source
gf	-34.84	kJ/mol	Joback Method
hf	-51.54	kJ/mol	Joback Method
hfus	9.90	kJ/mol	Joback Method
hvap	38.16	kJ/mol	Joback Method
ie	10.67 ± 0.02	eV	NIST Webbook
ie	10.40	eV	NIST Webbook
log10ws	-3.01		Crippen Method
logp	2.865		Crippen Method
mcvol	84.430	ml/mol	McGowan Method
pc	6599.09	kPa	Joback Method
rinpol	845.00		NIST Webbook
rinpol	843.00		NIST Webbook
tb	426.23	K	Joback Method
tc	672.87	K	Joback Method
tf	282.89	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.71	J/mol×K	508.44	Joback Method
cpg	104.97	J/mol×K	672.87	Joback Method

cpg	104.40	J/mol×K	631.76	Joback Method
cpg	103.55	J/mol×K	590.66	Joback Method
cpg	102.34	J/mol×K	549.55	Joback Method
cpg	95.93	J/mol×K	426.23	Joback Method
cpg	98.60	J/mol×K	467.34	Joback Method
dvisc	0.0024039	Pa×s	306.78	Joback Method
dvisc	0.0016658	Pa×s	330.67	Joback Method
dvisc	0.0012129	Pa×s	354.56	Joback Method
dvisc	0.0009192	Pa×s	378.45	Joback Method
dvisc	0.0007199	Pa×s	402.34	Joback Method
dvisc	0.0036906	Pa×s	282.89	Joback Method
dvisc	0.0005795	Pa×s	426.23	Joback Method
hfust	2.30	kJ/mol	294.40	NIST Webbook
hfust	5.40	kJ/mol	258.80	NIST Webbook
hfust	2.31	kJ/mol	294.40	NIST Webbook
sfust	7.90	J/mol×K	294.40	NIST Webbook
sfust	21.00	J/mol×K	258.80	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C594183&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: 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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

pc:	Critical Pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume