

Bromoacetyl bromide

Other names:	Acetyl bromide, bromo- UN 2513
Inchi:	InChI=1S/C2H2Br2O/c3-1-2(4)5/h1H2
InchiKey:	LSTRKXWIZZZYAS-UHFFFAOYSA-N
Formula:	C2H2Br2O
SMILES:	O=C(Br)CBr
Mol. weight [g/mol]:	201.84
CAS:	598-21-0

Physical Properties

Property code	Value	Unit	Source
gf	-134.32	kJ/mol	Joback Method
hf	-144.53	kJ/mol	Joback Method
hfus	13.10	kJ/mol	Joback Method
hvap	39.66	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	1.303		Crippen Method
mvol	75.610	ml/mol	McGowan Method
pc	6841.44	kPa	Joback Method
tb	421.70	K	NIST Webbook
tc	655.94	K	Joback Method
tf	281.83	K	Joback Method
vc	0.278	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	96.14	J/molxK	431.35	Joback Method
cpg	99.79	J/molxK	468.78	Joback Method
cpg	103.14	J/molxK	506.21	Joback Method
cpg	106.21	J/molxK	543.65	Joback Method
cpg	109.02	J/molxK	581.08	Joback Method
cpg	111.60	J/molxK	618.51	Joback Method
cpg	113.97	J/molxK	655.94	Joback Method

dvisc	0.0028647	Paxs	281.83	Joback Method
dvisc	0.0019612	Paxs	306.75	Joback Method
dvisc	0.0014213	Paxs	331.67	Joback Method
dvisc	0.0010774	Paxs	356.59	Joback Method
dvisc	0.0008469	Paxs	381.51	Joback Method
dvisc	0.0006856	Paxs	406.43	Joback Method
dvisc	0.0005688	Paxs	431.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C598210&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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