

Bromiodomethane

Other names:	Methane, bromiodo-
Inchi:	InChI=1S/CH2BrI/c2-1-3/h1H2
InchiKey:	TUDWMIUPYRKEFN-UHFFFAOYSA-N
Formula:	CH2BrI
SMILES:	BrCI
Mol. weight [g/mol]:	220.84
CAS:	557-68-6

Physical Properties

Property code	Value	Unit	Source
gf	29.98	kJ/mol	Joback Method
hf	39.23	kJ/mol	Joback Method
hfus	8.04	kJ/mol	Joback Method
hvap	33.63	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.774		Crippen Method
mcvol	68.270	ml/mol	McGowan Method
pc	6229.41	kPa	Joback Method
tb	381.58	K	Joback Method
tc	615.34	K	Joback Method
tf	274.00 ± 1.50	K	NIST Webbook
vc	0.241	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	66.47	J/mol×K	381.58	Joback Method
cpg	76.68	J/mol×K	576.38	Joback Method
cpg	75.07	J/mol×K	537.42	Joback Method
cpg	73.27	J/mol×K	498.46	Joback Method
cpg	71.26	J/mol×K	459.50	Joback Method
cpg	69.00	J/mol×K	420.54	Joback Method
cpg	78.12	J/mol×K	615.34	Joback Method
dvisc	0.0005381	Paxs	381.58	Joback Method

dvisc	0.0006635	Paxs	354.46	Joback Method
dvisc	0.0008469	Paxs	327.35	Joback Method
dvisc	0.0011299	Paxs	300.24	Joback Method
dvisc	0.0015962	Paxs	273.12	Joback Method
dvisc	0.0024333	Paxs	246.00	Joback Method
dvisc	0.0041179	Paxs	218.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C557686&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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