Methane, bromodiiodo-

Other names: Bromodiiodomethane
Inchi: InChI=1S/CHBrI2/c2-1(3)4/h1H
InchiKey: PTGIGXMFLYACDM-UHFFFAOYSA-N
Formula: CHBrI2
SMILES: BrC(I)I
Mol. weight [g/mol]: 346.73
CAS: 557-95-9

Physical Properties

Property code	Value	Unit	Source
gf	85.66	kJ/mol	Joback Method
hf	110.82	kJ/mol	Joback Method
hfus	8.92	kJ/mol	Joback Method
hvap	42.61	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.535		Crippen Method
mcvol	94.090	ml/mol	McGowan Method
pc	6093.99	kPa	Joback Method
tb	474.28	K	Joback Method
tc	760.17	K	Joback Method
tf	261.95	K	Joback Method
vc	0.324	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	88.53	J/mol×K	474.28	Joback Method
cpg	90.38	J/mol×K	521.93	Joback Method
cpg	91.83	J/mol×K	569.58	Joback Method
cpg	92.95	J/mol×K	617.23	Joback Method
cpg	93.80	J/mol×K	664.88	Joback Method
cpg	94.48	J/mol×K	712.53	Joback Method
cpg	95.05	J/mol×K	760.17	Joback Method
dvisc	0.0057262	Pa×s	261.95	Joback Method

dvisc	0.0029793	Pa×s	297.34	Joback Method
dvisc	0.0017812	Pa×s	332.73	Joback Method
dvisc	0.0011756	Pa×s	368.12	Joback Method
dvisc	0.0008346	Pa×s	403.50	Joback Method
dvisc	0.0006261	Pa×s	438.89	Joback Method
dvisc	0.0004903	Pa×s	474.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C557959&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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