Bromomethyl radical

Inchi: InChI=1S/CH2Br/c1-2/h1H2
InchiKey: AOJDZKCUAATBGE-UHFFFAOYSA-N
Formula: CH2Br
SMILES: [CH2]Br
Mol. weight [g/mol]: 93.93
CAS: 16519-97-4

Physical Properties

Property code	Value	Unit	Source
ea	1.94	eV	NIST Webbook
ea	0.97 ± 0.16	eV	NIST Webbook
ea	0.79 ± 0.14	eV	NIST Webbook
gf	24.24	kJ/mol	Joback Method
hf	18.17	kJ/mol	Joback Method
hfus	5.31	kJ/mol	Joback Method
hvap	24.11	kJ/mol	Joback Method
ie	8.61 ± 0.01	eV	NIST Webbook
ie	8.72 ± 0.01	eV	NIST Webbook
ie	8.34 ± 0.11	eV	NIST Webbook
ie	8.61 ± 0.01	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
log10ws	-0.78		Crippen Method
logp	1.173		Crippen Method
mcvol	40.300	ml/mol	McGowan Method
pc	6932.88	kPa	Joback Method
tb	287.74	K	Joback Method
tc	468.60	K	Joback Method
tf	177.20	K	Joback Method
vc	0.144	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	36.65	J/mol×K	287.74	Joback Method

cpg	39.43	J/mol×K	317.88	Joback Method
cpg	41.89	J/mol×K	348.03	Joback Method
cpg	44.07	J/mol×K	378.17	Joback Method
cpg	45.98	J/mol×K	408.32	Joback Method
cpg	47.64	J/mol×K	438.46	Joback Method
cpg	49.09	J/mol×K	468.60	Joback Method
dvisc	0.0005163	Pa×s	177.20	Joback Method
dvisc	0.0004556	Pa×s	195.62	Joback Method
dvisc	0.0004108	Pa×s	214.05	Joback Method
dvisc	0.0003765	Pa×s	232.47	Joback Method
dvisc	0.0003496	Pa×s	250.89	Joback Method
dvisc	0.0003279	Pa×s	269.32	Joback Method
dvisc	0.0003100	Pa×s	287.74	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=C16519974&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
ea: Electron affinity
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
ie: Ionization energy
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