

bromo(2H3)methane

Other names:	Methylbromide-d3
Inchi:	InChI=1S/CH3Br/c1-2/h1H3/i1D3
InchiKey:	GZUXJHMPEANEGY-FIBGUPNXSA-N
Formula:	CD3Br
SMILES:	CBr
Mol. weight [g/mol]:	97.96
CAS:	1111-88-2

Physical Properties

Property code	Value	Unit	Source
gf	-28.14	kJ/mol	Joback Method
hf	-37.64	kJ/mol	Joback Method
hfus	3.63	kJ/mol	Joback Method
hvap	24.26	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	1.011		Crippen Method
mcvol	42.450	ml/mol	McGowan Method
pc	6451.51	kPa	Joback Method
tb	288.44	K	Joback Method
tc	473.09	K	Joback Method
tf	160.83	K	Joback Method
vc	0.153	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	42.04	J/molxK	288.44	Joback Method
cpg	53.83	J/molxK	442.32	Joback Method
cpg	51.71	J/molxK	411.54	Joback Method
cpg	49.48	J/molxK	380.77	Joback Method
cpg	47.12	J/molxK	349.99	Joback Method
cpg	44.65	J/molxK	319.22	Joback Method
cpg	55.85	J/molxK	473.09	Joback Method
dvisc	0.0003302	Paxs	288.44	Joback Method

dvisc	0.0003994	Paxs	267.17	Joback Method
dvisc	0.0004993	Paxs	245.90	Joback Method
dvisc	0.0006511	Paxs	224.63	Joback Method
dvisc	0.0008975	Paxs	203.37	Joback Method
dvisc	0.0013334	Paxs	182.10	Joback Method
dvisc	0.0021998	Paxs	160.83	Joback Method

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=C1111882&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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