

1,3-bromomethoxypropane

Inchi:	InChI=1S/C4H9BrO/c1-6-4-2-3-5/h2-4H2,1H3
InchiKey:	CEVMYGZHEJSOHZ-UHFFFAOYSA-N
Formula:	C4H9BrO
SMILES:	COCCCBBr
Mol. weight [g/mol]:	153.02

Physical Properties

Property code	Value	Unit	Source
gf	-107.88	kJ/mol	Joback Method
hf	-231.78	kJ/mol	Joback Method
hfus	12.59	kJ/mol	Joback Method
hvap	33.34	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	1.418		Crippen Method
mcvol	90.590	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
rinpol	823.10		NIST Webbook
tb	379.50	K	Joback Method
tc	565.42	K	Joback Method
tf	216.87	K	Joback Method
vc	0.340	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.77	J/molxK	379.50	Joback Method
cpg	155.34	J/molxK	410.49	Joback Method
cpg	162.65	J/molxK	441.47	Joback Method
cpg	169.71	J/molxK	472.46	Joback Method
cpg	176.51	J/molxK	503.44	Joback Method
cpg	183.06	J/molxK	534.43	Joback Method
cpg	189.37	J/molxK	565.42	Joback Method
dvisc	0.0028309	Paxs	216.87	Joback Method
dvisc	0.0016164	Paxs	243.97	Joback Method

dvisc	0.0010324	Paxs	271.08	Joback Method
dvisc	0.0007153	Paxs	298.19	Joback Method
dvisc	0.0005269	Paxs	325.29	Joback Method
dvisc	0.0004068	Paxs	352.39	Joback Method
dvisc	0.0003259	Paxs	379.50	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=R135830&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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