

3-Bromo-2-methoxypropene

Inchi:	InChI=1S/C4H7BrO/c1-4(3-5)6-2/h1,3H2,2H3
InchiKey:	MALRJHQIKRJCMN-UHFFFAOYSA-N
Formula:	C4H7BrO
SMILES:	C=C(CBr)OC
Mol. weight [g/mol]:	151.00

Physical Properties

Property code	Value	Unit	Source
gf	-28.59	kJ/mol	Joback Method
hf	-116.14	kJ/mol	Joback Method
hfus	10.00	kJ/mol	Joback Method
hvap	32.75	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.541		Crippen Method
mcvol	86.290	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
ripol	1095.00		NIST Webbook
ripol	1095.00		NIST Webbook
tb	376.06	K	Joback Method
tc	570.07	K	Joback Method
tf	201.15	K	Joback Method
vc	0.322	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	134.13	J/mol×K	376.06	Joback Method
cpg	141.05	J/mol×K	408.40	Joback Method
cpg	147.69	J/mol×K	440.73	Joback Method
cpg	154.04	J/mol×K	473.07	Joback Method
cpg	160.13	J/mol×K	505.40	Joback Method
cpg	165.95	J/mol×K	537.74	Joback Method
cpg	171.52	J/mol×K	570.07	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=R593934&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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