Hexane, 1-bromo-2-methoxy

Inchi: InChI=1S/C7H15BrO/c1-3-4-5-7(6-8)9-2/h7H,3-6H2,1-2H3
InchiKey: CCRWCKSQBQNHJC-UHFFFAOYSA-N
Formula: C7H15BrO
SMILES: CCCCC(CBr)OC
Mol. weight [g/mol]: 195.10

Physical Properties

Property code	Value	Unit	Source
gf	-85.06	kJ/mol	Joback Method
hf	-298.98	kJ/mol	Joback Method
hfus	16.84	kJ/mol	Joback Method
hvap	39.63	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.587		Crippen Method
mcvol	132.860	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpol	1032.00		NIST Webbook
tb	447.70	K	Joback Method
tc	633.73	K	Joback Method
tf	235.68	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.73	J/mol×K	447.70	Joback Method
cpg	271.68	J/mol×K	478.71	Joback Method
cpg	283.16	J/mol×K	509.71	Joback Method
cpg	294.17	J/mol×K	540.72	Joback Method
cpg	304.72	J/mol×K	571.72	Joback Method
cpg	314.83	J/mol×K	602.73	Joback Method
cpg	324.49	J/mol×K	633.73	Joback Method
dvisc	0.0045222	Pa×s	235.68	Joback Method
dvisc	0.0020680	Pa×s	271.02	Joback Method

dvisc	0.0011328	Pa×s	306.35	Joback Method
dvisc	0.0007028	Pa×s	341.69	Joback Method
dvisc	0.0004768	Pa×s	377.03	Joback Method
dvisc	0.0003457	Pa×s	412.36	Joback Method
dvisc	0.0002637	Pa×s	447.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R12006&Units=SI

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