Pentane, 1-bromo-2-methoxy

Inchi: InChI=1S/C6H13BrO/c1-3-4-6(5-7)8-2/h6H,3-5H2,1-2H3
InchiKey: JDAILCRIKVLCFU-UHFFFAOYSA-N
Formula: C6H13BrO
SMILES: CCCC(CBr)OC
Mol. weight [g/mol]: 181.07

Physical Properties

Property code	Value	Unit	Source
gf	-93.48	kJ/mol	Joback Method
hf	-278.34	kJ/mol	Joback Method
hfus	14.25	kJ/mol	Joback Method
hvap	37.41	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	2.196		Crippen Method
mcvol	118.770	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	936.00		NIST Webbook
rinpol	936.00		NIST Webbook
tb	424.82	K	Joback Method
tc	612.54	K	Joback Method
tf	224.41	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.06	J/mol×K	424.82	Joback Method
cpg	269.61	J/mol×K	581.26	Joback Method
cpg	260.50	J/mol×K	549.97	Joback Method
cpg	251.00	J/mol×K	518.68	Joback Method
cpg	241.10	J/mol×K	487.39	Joback Method
cpg	230.79	J/mol×K	456.11	Joback Method
cpg	278.33	J/mol×K	612.54	Joback Method
dvisc	0.0002837	Pa×s	424.82	Joback Method

dvisc	0.0003698	Pa×s	391.42	Joback Method
dvisc	0.0005066	Pa×s	358.02	Joback Method
dvisc	0.0007403	Pa×s	324.62	Joback Method
dvisc	0.0011802	Pa×s	291.21	Joback Method
dvisc	0.0021234	Pa×s	257.81	Joback Method
dvisc	0.0045501	Pa×s	224.41	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=R12024&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