Pentane, 3-bromo-2-methoxy, erythro

Inchi: InChI=1S/C6H13BrO/c1-4-6(7)5(2)8-3/h5-6H,4H2,1-3H3/t5-,6+/m1/s1
InchiKey: HZOOMUCVVMOMOV-RITPCOANSA-N
Formula: C6H13BrO
SMILES: CCC(Br)C(C)OC
Mol. weight [g/mol]: 181.07

Physical Properties

Property code	Value	Unit	Source
gf	-95.92	kJ/mol	Joback Method
hf	-283.62	kJ/mol	Joback Method
hfus	10.72	kJ/mol	Joback Method
hvap	37.02	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	2.195		Crippen Method
mcvol	118.770	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	914.00		NIST Webbook
rinpol	914.00		NIST Webbook
tb	424.38	K	Joback Method
tc	616.51	K	Joback Method
tf	209.41	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.12	J/mol×K	424.38	Joback Method
cpg	271.11	J/mol×K	584.49	Joback Method
cpg	261.77	J/mol×K	552.47	Joback Method
cpg	252.01	J/mol×K	520.45	Joback Method
cpg	241.82	J/mol×K	488.42	Joback Method
cpg	231.19	J/mol×K	456.40	Joback Method
cpg	280.04	J/mol×K	616.51	Joback Method
dvisc	0.0002721	Pa×s	424.38	Joback Method

dvisc	0.0003655	Pa×s	388.55	Joback Method
dvisc	0.0005212	Pa×s	352.72	Joback Method
dvisc	0.0008055	Pa×s	316.89	Joback Method
dvisc	0.0013909	Pa×s	281.07	Joback Method
dvisc	0.0028172	Pa×s	245.24	Joback Method
dvisc	0.0072653	Pa×s	209.41	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=R294692&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