

Pentane, 2-bromo-3-methoxy, threo

Inchi:	InChI=1S/C6H13BrO/c1-4-6(8-3)5(2)7/h5-6H,4H2,1-3H3/t5-,6-/m0/s1
InchiKey:	YHELFDGYBWOBGG-WDSKDSINSA-N
Formula:	C6H13BrO
SMILES:	CCC(OC)C(C)Br
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	906.00		NIST Webbook
tb	424.38	K	Joback Method
tc	616.51	K	Joback Method
tf	209.41	K	Joback Method
vc	0.440	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.12	J/molxK	424.38	Joback Method
cpg	231.19	J/molxK	456.40	Joback Method
cpg	241.82	J/molxK	488.42	Joback Method
cpg	252.01	J/molxK	520.45	Joback Method
cpg	261.77	J/molxK	552.47	Joback Method
cpg	271.11	J/molxK	584.49	Joback Method
cpg	280.04	J/molxK	616.51	Joback Method
dvisc	0.0072653	Paxs	209.41	Joback Method
dvisc	0.0028172	Paxs	245.24	Joback Method

dvisc	0.0013909	Paxs	281.07	Joback Method
dvisc	0.0008055	Paxs	316.89	Joback Method
dvisc	0.0005212	Paxs	352.72	Joback Method
dvisc	0.0003655	Paxs	388.55	Joback Method
dvisc	0.0002721	Paxs	424.38	Joback Method

Sources

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=R294687&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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