

Hexane, 2-bromo-3-methoxy, threo

Inchi:	InChI=1S/C7H15BrO/c1-4-5-7(9-3)6(2)8/h6-7H,4-5H2,1-3H3/t6-,7-/m0/s1
InchiKey:	SHKMJZCDMYBQGL-BQBZGAKWSA-N
Formula:	C7H15BrO
SMILES:	CCCC(OC)C(C)Br
Mol. weight [g/mol]:	195.10

Physical Properties

Property code	Value	Unit	Source
gf	-87.50	kJ/mol	Joback Method
hf	-304.26	kJ/mol	Joback Method
hfus	13.31	kJ/mol	Joback Method
hvap	39.25	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.585		Crippen Method
mcvol	132.860	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	990.00		NIST Webbook
rinpol	990.00		NIST Webbook
tb	447.26	K	Joback Method
tc	637.53	K	Joback Method
tf	220.68	K	Joback Method
vc	0.495	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.84	J/molxK	447.26	Joback Method
cpg	272.15	J/molxK	478.97	Joback Method
cpg	283.95	J/molxK	510.68	Joback Method
cpg	295.26	J/molxK	542.40	Joback Method
cpg	306.08	J/molxK	574.11	Joback Method
cpg	316.43	J/molxK	605.82	Joback Method
cpg	326.31	J/molxK	637.53	Joback Method
dvisc	0.0070586	Paxs	220.68	Joback Method

dvisc	0.0026988	Paxs	258.44	Joback Method
dvisc	0.0013185	Paxs	296.21	Joback Method
dvisc	0.0007574	Paxs	333.97	Joback Method
dvisc	0.0004870	Paxs	371.73	Joback Method
dvisc	0.0003397	Paxs	409.50	Joback Method
dvisc	0.0002518	Paxs	447.26	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=R294627&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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