Hexane, 2-bromo-3-methoxy, erythro

Inchi: InChI=1S/C7H15BrO/c1-4-5-7(9-3)6(2)8/h6-7H,4-5H2,1-3H3/t6-,7+/m1/s1
InchiKey: SHKMJZCDMYBQGL-RQJHMYQMSA-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	991.00		NIST Webbook
rinpol	991.00		NIST Webbook
tb	447.26	K	Joback Method
tc	637.53	K	Joback Method
tf	220.68	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0026988	Pa×s	258.44	Joback Method
dvisc	0.0013185	Pa×s	296.21	Joback Method
dvisc	0.0007574	Pa×s	333.97	Joback Method
dvisc	0.0004870	Pa×s	371.73	Joback Method
dvisc	0.0003397	Pa×s	409.50	Joback Method
dvisc	0.0002518	Pa×s	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=R294612&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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