5-Bromovaleric acid, tridecyl ester

Inchi: InChI=1S/C18H35BrO2/c1-2-3-4-5-6-7-8-9-10-11-14-17-21-18(20)15-12-13-16-19/h2-17
InchiKey: HVGBJOBIODVPDH-UHFFFAOYSA-N
Formula: C18H35BrO2
SMILES: CCCCCCCCCCCCCOC(=O)CCCCBr
Mol. weight [g/mol]: 363.37

Physical Properties

Property code	Value	Unit	Source
gf	-118.92	kJ/mol	Joback Method
hf	-633.32	kJ/mol	Joback Method
hfus	50.45	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	6.406		Crippen Method
mcvol	289.420	ml/mol	McGowan Method
pc	1247.73	kPa	Joback Method
rinpol	2351.30		NIST Webbook
tb	753.69	K	Joback Method
tc	933.68	K	Joback Method
tf	424.58	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.90	J/mol×K	753.69	Joback Method
cpg	923.68	J/mol×K	903.68	Joback Method
cpg	909.38	J/mol×K	873.69	Joback Method
cpg	894.28	J/mol×K	843.69	Joback Method
cpg	878.35	J/mol×K	813.69	Joback Method
cpg	861.56	J/mol×K	783.69	Joback Method
cpg	937.22	J/mol×K	933.68	Joback Method
dvisc	0.0000782	Pa×s	753.69	Joback Method
dvisc	0.0001031	Pa×s	698.84	Joback Method

dvisc	0.0001426	Pa×s	643.99	Joback Method
dvisc	0.0002094	Pa×s	589.13	Joback Method
dvisc	0.0003328	Pa×s	534.28	Joback Method
dvisc	0.0005881	Pa×s	479.43	Joback Method
dvisc	0.0012037	Pa×s	424.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292290&Units=SI
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

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