Undecyl 5-bromovalerate

Other names: 5-Bromovaleric acid, undecyl ester
Inchi: InChI=1S/C16H31BrO2/c1-2-3-4-5-6-7-8-9-12-15-19-16(18)13-10-11-14-17/h2-15H2,1H3
InchiKey: MWDGQCNABWWJEF-UHFFFAOYSA-N
Formula: C16H31BrO2
SMILES: CCCCCCCCCCCOC(=O)CCCCBr
Mol. weight [g/mol]: 335.32
CAS: 300381-07-1

Physical Properties

Property code	Value	Unit	Source
gf	-135.76	kJ/mol	Joback Method
hf	-592.04	kJ/mol	Joback Method
hfus	45.27	kJ/mol	Joback Method
hvap	66.80	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.626		Crippen Method
mcvol	261.240	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	2122.00		NIST Webbook
rinpol	2122.00		NIST Webbook
tb	707.93	K	Joback Method
tc	886.70	K	Joback Method
tf	402.04	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.59	J/mol×K	707.93	Joback Method
cpg	745.44	J/mol×K	737.72	Joback Method
cpg	761.48	J/mol×K	767.52	Joback Method
cpg	776.72	J/mol×K	797.31	Joback Method
cpg	791.21	J/mol×K	827.11	Joback Method
cpg	804.95	J/mol×K	856.90	Joback Method

cpg	817.97	J/mol×K	886.70	Joback Method
dvisc	0.0014706	Pa×s	402.04	Joback Method
dvisc	0.0007366	Pa×s	453.02	Joback Method
dvisc	0.0004243	Pa×s	504.00	Joback Method
dvisc	0.0002705	Pa×s	554.99	Joback Method
dvisc	0.0001860	Pa×s	605.97	Joback Method
dvisc	0.0001356	Pa×s	656.95	Joback Method
dvisc	0.0001034	Pa×s	707.93	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=C300381071&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

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