5-Bromovaleric acid, 3-tridecyl ester

Inchi: InChI=1S/C18H35BrO2/c1-3-5-6-7-8-9-10-11-14-17(4-2)21-18(20)15-12-13-16-19/h17H,
InchiKey: DBWYEIHZSBBMFC-UHFFFAOYSA-N
Formula: C18H35BrO2
SMILES: CCCCCCCCCCC(CC)OC(=O)CCCCBr
Mol. weight [g/mol]: 363.37

Physical Properties

Property code	Value	Unit	Source
gf	-121.36	kJ/mol	Joback Method
hf	-638.60	kJ/mol	Joback Method
hfus	46.92	kJ/mol	Joback Method
hvap	70.86	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.404		Crippen Method
mcvol	289.420	ml/mol	McGowan Method
pc	1254.81	kPa	Joback Method
rinpol	2191.00		NIST Webbook
rinpol	2191.00		NIST Webbook
tb	753.25	K	Joback Method
tc	934.86	K	Joback Method
tf	409.58	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.38	J/mol×K	753.25	Joback Method
cpg	862.22	J/mol×K	783.52	Joback Method
cpg	879.15	J/mol×K	813.79	Joback Method
cpg	895.20	J/mol×K	844.05	Joback Method
cpg	910.40	J/mol×K	874.32	Joback Method
cpg	924.79	J/mol×K	904.59	Joback Method
cpg	938.38	J/mol×K	934.86	Joback Method
dvisc	0.0014522	Pa×s	409.58	Joback Method

dvisc	0.0006475	Pa×s	466.86	Joback Method
dvisc	0.0003445	Pa×s	524.14	Joback Method
dvisc	0.0002075	Pa×s	581.41	Joback Method
dvisc	0.0001369	Pa×s	638.69	Joback Method
dvisc	0.0000967	Pa×s	695.97	Joback Method
dvisc	0.0000721	Pa×s	753.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299925&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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