

5-Bromovaleric acid, 3-tetradecyl ester

Inchi:

lnchl=1S/C19H37BrO2/c1-3-5-6-7-8-9-10-11-12-15-18(4-2)22-19(21)16-13-14-17-20/h1

InchiKey:

NFOMVCBZZCAPMC-UHFFFAOYSA-N

Formula:

C19H37BrO2

SMILES:

CCCCCCCCCCCC(CC)OC(=O)CCCCBr

Mol. weight [g/mol]:

377.40

Physical Properties

Property code	Value	Unit	Source
gf	-112.94	kJ/mol	Joback Method
hf	-659.24	kJ/mol	Joback Method
hfus	49.51	kJ/mol	Joback Method
hvap	73.09	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.794		Crippen Method
mcvol	303.510	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpol	2297.00		NIST Webbook
tb	776.13	K	Joback Method
tc	958.94	K	Joback Method
tf	420.85	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.57	J/mol×K	776.13	Joback Method
cpg	985.51	J/mol×K	928.48	Joback Method
cpg	970.88	J/mol×K	898.01	Joback Method
cpg	955.40	J/mol×K	867.54	Joback Method
cpg	939.05	J/mol×K	837.07	Joback Method
cpg	921.78	J/mol×K	806.60	Joback Method
cpg	999.32	J/mol×K	958.94	Joback Method
dvisc	0.0000623	Pa×s	776.13	Joback Method
dvisc	0.0000838	Pa×s	716.92	Joback Method

dvisc	0.0001190	Pa×s	657.70	Joback Method
dvisc	0.0001811	Pa×s	598.49	Joback Method
dvisc	0.0003022	Pa×s	539.28	Joback Method
dvisc	0.0005721	Pa×s	480.06	Joback Method
dvisc	0.0012961	Pa×s	420.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299929&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

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