

5-Bromovaleric acid, 4-tetradecyl ester

Inchi:	InChI=1S/C19H37BrO2/c1-3-5-6-7-8-9-10-11-15-18(14-4-2)22-19(21)16-12-13-17-20/h1
InchiKey:	CGIVVZRJFQNHVDV-UHFFFAOYSA-N
Formula:	C19H37BrO2
SMILES:	CCCCCCCCCCC(CCC)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
mvol	303.510	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rmpol	2269.00		NIST Webbook
tb	776.13	K	Joback Method
tc	958.94	K	Joback Method
tf	420.85	K	Joback Method
vc	1.179	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.57	J/molxK	776.13	Joback Method
cpg	921.78	J/molxK	806.60	Joback Method
cpg	939.05	J/molxK	837.07	Joback Method
cpg	955.40	J/molxK	867.54	Joback Method
cpg	970.88	J/molxK	898.01	Joback Method
cpg	985.51	J/molxK	928.48	Joback Method
cpg	999.32	J/molxK	958.94	Joback Method
dvisc	0.0012961	Paxs	420.85	Joback Method
dvisc	0.0005721	Paxs	480.06	Joback Method

dvisc	0.0003022	Paxs	539.28	Joback Method
dvisc	0.0001811	Paxs	598.49	Joback Method
dvisc	0.0001190	Paxs	657.70	Joback Method
dvisc	0.0000838	Paxs	716.92	Joback Method
dvisc	0.0000623	Paxs	776.13	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=U299930&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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