

5-Bromovaleric acid, tetradecyl ester

Inchi:	InChI=1S/C19H37BrO2/c1-2-3-4-5-6-7-8-9-10-11-12-15-18-22-19(21)16-13-14-17-20/h2
InchiKey:	GBDPMICJPHVMCS-UHFFFAOYSA-N
Formula:	C19H37BrO2
SMILES:	CCCCCCCCCCCCCOC(=O)CCCCBr
Mol. weight [g/mol]:	377.40

Physical Properties

Property code	Value	Unit	Source
gf	-110.50	kJ/mol	Joback Method
hf	-653.96	kJ/mol	Joback Method
hfus	53.04	kJ/mol	Joback Method
hvap	73.48	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	6.796		Crippen Method
mcvol	303.510	ml/mol	McGowan Method
pc	1167.22	kPa	Joback Method
rinpol	2451.20		NIST Webbook
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tb	776.57	K	Joback Method
tc	958.06	K	Joback Method
tf	435.85	K	Joback Method
vc	1.185	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.09	J/molxK	776.57	Joback Method
cpg	921.16	J/molxK	806.82	Joback Method
cpg	938.31	J/molxK	837.07	Joback Method
cpg	954.57	J/molxK	867.31	Joback Method
cpg	969.97	J/molxK	897.56	Joback Method
cpg	984.54	J/molxK	927.81	Joback Method
cpg	998.31	J/molxK	958.06	Joback Method
dvisc	0.0010816	Paxs	435.85	Joback Method

dvisc	0.0005223	Paxs	492.64	Joback Method
dvisc	0.0002932	Paxs	549.42	Joback Method
dvisc	0.0001834	Paxs	606.21	Joback Method
dvisc	0.0001243	Paxs	663.00	Joback Method
dvisc	0.0000896	Paxs	719.78	Joback Method
dvisc	0.0000677	Paxs	776.57	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=U292291&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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