

2-Bromotetradecanoic acid

Other names:	Tetradecanoic acid, 2-bromo- «alpha»-Bromomyristic acid
Inchi:	InChI=1S/C14H27BrO2/c1-2-3-4-5-6-7-8-9-10-11-12-13(15)14(16)17/h13H,2-12H2,1H3,
InchiKey:	GBBKJNDQLLKTCX-UHFFFAOYSA-N
Formula:	C14H27BrO2
SMILES:	CCCCCCCCCCCCC(Br)C(=O)O
Mol. weight [g/mol]:	307.27
CAS:	10520-81-7

Physical Properties

Property code	Value	Unit	Source
gf	-186.86	kJ/mol	Joback Method
hf	-576.05	kJ/mol	Joback Method
hfus	39.47	kJ/mol	Joback Method
hvap	76.23	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	5.146		Crippen Method
mvol	233.060	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
tb	731.49	K	Joback Method
tc	911.27	K	Joback Method
tf	403.09	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.96	J/molxK	731.49	Joback Method
cpg	669.07	J/molxK	761.45	Joback Method
cpg	682.47	J/molxK	791.42	Joback Method
cpg	695.21	J/molxK	821.38	Joback Method
cpg	707.31	J/molxK	851.34	Joback Method
cpg	718.79	J/molxK	881.31	Joback Method
cpg	729.70	J/molxK	911.27	Joback Method

dvisc	0.0026780	Paxs	403.09	Joback Method
dvisc	0.0008380	Paxs	457.82	Joback Method
dvisc	0.0003361	Paxs	512.56	Joback Method
dvisc	0.0001608	Paxs	567.29	Joback Method
dvisc	0.0000876	Paxs	622.02	Joback Method
dvisc	0.0000526	Paxs	676.76	Joback Method
dvisc	0.0000341	Paxs	731.49	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C10520817&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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