2- Bromopropionic acid, tetradecyl ester

Other names: Tetradecyl 2-bromopropanoate
Inchi: InChI=1S/C17H33BrO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-20-17(19)16(2)18/h16H,3-1
InchiKey: XLNAEONRIMSMIY-UHFFFAOYSA-N
Formula: C17H33BrO2
SMILES: CCCCCCCCCCCCCCOC(=O)C(C)Br
Mol. weight [g/mol]: 349.35
CAS: 86711-82-2

Physical Properties

Property code	Value	Unit	Source
gf	-129.78	kJ/mol	Joback Method
hf	-617.96	kJ/mol	Joback Method
hfus	44.34	kJ/mol	Joback Method
hvap	68.64	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	6.014		Crippen Method
mcvol	275.330	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rinpol	2140.40		NIST Webbook
rinpol	2140.40		NIST Webbook
rinpol	2111.00		NIST Webbook
rinpol	2111.00		NIST Webbook
tb	730.37	K	Joback Method
tc	911.36	K	Joback Method
tf	398.31	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.19	J/mol×K	730.37	Joback Method
cpg	803.65	J/mol×K	760.54	Joback Method
cpg	820.24	J/mol×K	790.70	Joback Method
cpg	835.98	J/mol×K	820.87	Joback Method

cpg	850.90	J/mol×K	851.03	Joback Method
cpg	865.04	J/mol×K	881.20	Joback Method
cpg	878.40	J/mol×K	911.36	Joback Method
dvisc	0.0016202	Pa×s	398.31	Joback Method
dvisc	0.0007302	Pa×s	453.65	Joback Method
dvisc	0.0003914	Pa×s	509.00	Joback Method
dvisc	0.0002371	Pa×s	564.34	Joback Method
dvisc	0.0001571	Pa×s	619.68	Joback Method
dvisc	0.0001113	Pa×s	675.03	Joback Method
dvisc	0.0000831	Pa×s	730.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86711822&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

Latest version available from: