

Bromoacetic acid, hexadecyl ester

Other names:	Hexadecyl bromoacetate
Inchi:	InChI=1S/C18H35BrO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-18(20)17-19/h2-17
InchiKey:	BTHNTCJTOYZMCB-UHFFFAOYSA-N
Formula:	C18H35BrO2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CBr
Mol. weight [g/mol]:	363.37
CAS:	5454-48-8

Physical Properties

Property code	Value	Unit	Source
gf	-118.92	kJ/mol	Joback Method
hf	-633.32	kJ/mol	Joback Method
hfus	50.45	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	6.406		Crippen Method
mcvol	289.420	ml/mol	McGowan Method
pc	1247.73	kPa	Joback Method
rinpol	2287.60		NIST Webbook
tb	753.69	K	Joback Method
tc	933.68	K	Joback Method
tf	424.58	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.90	J/molxK	753.69	Joback Method
cpg	861.56	J/molxK	783.69	Joback Method
cpg	878.35	J/molxK	813.69	Joback Method
cpg	894.28	J/molxK	843.69	Joback Method
cpg	909.38	J/molxK	873.69	Joback Method
cpg	923.68	J/molxK	903.68	Joback Method
cpg	937.22	J/molxK	933.68	Joback Method

dvisc	0.0012037	Paxs	424.58	Joback Method
dvisc	0.0005881	Paxs	479.43	Joback Method
dvisc	0.0003328	Paxs	534.28	Joback Method
dvisc	0.0002094	Paxs	589.13	Joback Method
dvisc	0.0001426	Paxs	643.99	Joback Method
dvisc	0.0001031	Paxs	698.84	Joback Method
dvisc	0.0000782	Paxs	753.69	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=C5454488&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
mvol:	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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