

2- Bromopropionic acid, octadecyl ester

Inchi:	InChI=1S/C21H41BrO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-21(23)20(2)
InchiKey:	KPORSMDXMDNWRZ-UHFFFAOYSA-N
Formula:	C21H41BrO2
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(C)Br
Mol. weight [g/mol]:	405.45
CAS:	89876-55-1

Physical Properties

Property code	Value	Unit	Source
gf	-96.10	kJ/mol	Joback Method
hf	-700.52	kJ/mol	Joback Method
hfus	54.70	kJ/mol	Joback Method
hvap	77.54	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	7.575		Crippen Method
mcvol	331.690	ml/mol	McGowan Method
pc	1033.24	kPa	Joback Method
rinpol	2548.60		NIST Webbook
tb	821.89	K	Joback Method
tc	1009.13	K	Joback Method
tf	443.39	K	Joback Method
vc	1.292	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.62	J/molxK	821.89	Joback Method
cpg	1043.63	J/molxK	853.10	Joback Method
cpg	1061.60	J/molxK	884.30	Joback Method
cpg	1078.58	J/molxK	915.51	Joback Method
cpg	1094.61	J/molxK	946.72	Joback Method
cpg	1109.71	J/molxK	977.92	Joback Method
cpg	1123.94	J/molxK	1009.13	Joback Method
dvisc	0.0010210	Paxs	443.39	Joback Method

dvisc	0.0004422	Paxs	506.47	Joback Method
dvisc	0.0002305	Paxs	569.56	Joback Method
dvisc	0.0001368	Paxs	632.64	Joback Method
dvisc	0.0000893	Paxs	695.72	Joback Method
dvisc	0.0000626	Paxs	758.81	Joback Method
dvisc	0.0000463	Paxs	821.89	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=C89876551&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
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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