2- Bromopropionic acid, hexadecyl ester

Other names: Hexadecyl 2-bromopropanoate
Inchi: InChI=1S/C19H37BrO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-19(21)18(2)20/h18
InchiKey: LOGGHEZVYPCZGT-UHFFFAOYSA-N
Formula: C19H37BrO2
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)Br
Mol. weight [g/mol]: 377.40
CAS: 63966-83-6

Physical Properties

Property code	Value	Unit	Source
gf	-112.94	kJ/mol	Joback Method
hf	-659.24	kJ/mol	Joback Method
hfus	49.51	kJ/mol	Joback Method
hvap	73.09	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.794		Crippen Method
mcvol	303.510	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpol	2312.00		NIST Webbook
rinpol	2312.00		NIST Webbook
rinpol	2343.50		NIST Webbook
tb	776.13	K	Joback Method
tc	958.94	K	Joback Method
tf	420.85	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.57	J/mol×K	776.13	Joback Method
cpg	921.78	J/mol×K	806.60	Joback Method
cpg	939.05	J/mol×K	837.07	Joback Method
cpg	955.40	J/mol×K	867.54	Joback Method
cpg	970.88	J/mol×K	898.01	Joback Method

cpg	985.51	J/mol×K	928.48	Joback Method
cpg	999.32	J/mol×K	958.94	Joback Method
dvisc	0.0012961	Pa×s	420.85	Joback Method
dvisc	0.0005721	Pa×s	480.06	Joback Method
dvisc	0.0003022	Pa×s	539.28	Joback Method
dvisc	0.0001811	Pa×s	598.49	Joback Method
dvisc	0.0001190	Pa×s	657.70	Joback Method
dvisc	0.0000838	Pa×s	716.92	Joback Method
dvisc	0.0000623	Pa×s	776.13	Joback Method

Sources

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=C63966836&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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