Hexadecyl 2-bromobutanoate

Inchi: InChI=1S/C20H39BrO2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-20(22)19(21)4-2/
InchiKey: DWBJZRRQROSBIE-UHFFFAOYSA-N
Formula: C20H39BrO2
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(Br)CC
Mol. weight [g/mol]: 391.43

Physical Properties

Property code	Value	Unit	Source
gf	-104.52	kJ/mol	Joback Method
hf	-679.88	kJ/mol	Joback Method
hfus	52.10	kJ/mol	Joback Method
hvap	75.32	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	7.184		Crippen Method
mcvol	317.600	ml/mol	McGowan Method
pc	1100.08	kPa	Joback Method
rinpol	2399.00		NIST Webbook
rinpol	2399.00		NIST Webbook
tb	799.01	K	Joback Method
tc	983.68	K	Joback Method
tf	432.12	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.67	J/mol×K	799.01	Joback Method
cpg	1047.16	J/mol×K	952.90	Joback Method
cpg	1032.29	J/mol×K	922.13	Joback Method
cpg	1016.54	J/mol×K	891.35	Joback Method
cpg	999.88	J/mol×K	860.57	Joback Method
cpg	982.27	J/mol×K	829.79	Joback Method
cpg	1061.18	J/mol×K	983.68	Joback Method
dvisc	0.0000538	Pa×s	799.01	Joback Method

dvisc	0.0000725	Pa×s	737.86	Joback Method
dvisc	0.0001032	Pa×s	676.71	Joback Method
dvisc	0.0001576	Pa×s	615.57	Joback Method
dvisc	0.0002643	Pa×s	554.42	Joback Method
dvisc	0.0005038	Pa×s	493.27	Joback Method
dvisc	0.0011524	Pa×s	432.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R23401&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