5-Bromovaleric acid, pentadecyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-102.08	kJ/mol	Joback Method
hf	-674.60	kJ/mol	Joback Method
hfus	55.63	kJ/mol	Joback Method
hvap	75.70	kJ/mol	Joback Method
log10ws	-7.49		Crippen Method
logp	7.186		Crippen Method
mcvol	317.600	ml/mol	McGowan Method
pc	1094.27	kPa	Joback Method
rinpol	2547.20		NIST Webbook
rinpol	2547.20		NIST Webbook
tb	799.45	K	Joback Method
tc	983.10	K	Joback Method
tf	447.12	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.19	J/mol×K	799.45	Joback Method
cpg	1046.34	J/mol×K	952.49	Joback Method
cpg	1031.51	J/mol×K	921.88	Joback Method
cpg	1015.81	J/mol×K	891.27	Joback Method
cpg	999.21	J/mol×K	860.67	Joback Method
cpg	981.68	J/mol×K	830.06	Joback Method
cpg	1060.35	J/mol×K	983.10	Joback Method
dvisc	0.0000585	Pa×s	799.45	Joback Method

dvisc	0.0000776	Pa×s	740.73	Joback Method
dvisc	0.0001080	Pa×s	682.01	Joback Method
dvisc	0.0001601	Pa×s	623.28	Joback Method
dvisc	0.0002574	Pa×s	564.56	Joback Method
dvisc	0.0004622	Pa×s	505.84	Joback Method
dvisc	0.0009678	Pa×s	447.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292292&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