5-Bromovaleric acid, heptadecyl ester

Inchi: InChI=1S/C22H43BrO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-25-22(24)19-16-17-
InchiKey: QMVPPALRXHRWRX-UHFFFAOYSA-N
Formula: C22H43BrO2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCCBr
Mol. weight [g/mol]: 419.48

Physical Properties

Property code	Value	Unit	Source
gf	-85.24	kJ/mol	Joback Method
hf	-715.88	kJ/mol	Joback Method
hfus	60.81	kJ/mol	Joback Method
hvap	80.16	kJ/mol	Joback Method
log10ws	-8.33		Crippen Method
logp	7.966		Crippen Method
mcvol	345.780	ml/mol	McGowan Method
pc	967.47	kPa	Joback Method
rinpol	2749.00		NIST Webbook
rinpol	2749.00		NIST Webbook
tb	845.21	K	Joback Method
tc	1035.40	K	Joback Method
tf	469.66	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.90	J/mol×K	845.21	Joback Method
cpg	1105.31	J/mol×K	876.91	Joback Method
cpg	1123.66	J/mol×K	908.61	Joback Method
cpg	1140.97	J/mol×K	940.31	Joback Method
cpg	1157.29	J/mol×K	972.01	Joback Method
cpg	1172.67	J/mol×K	1003.71	Joback Method
cpg	1187.14	J/mol×K	1035.40	Joback Method
dvisc	0.0007664	Pa×s	469.66	Joback Method

dvisc	0.0003584	Pa×s	532.25	Joback Method
dvisc	0.0001967	Pa×s	594.84	Joback Method
dvisc	0.0001210	Pa×s	657.43	Joback Method
dvisc	0.0000810	Pa×s	720.03	Joback Method
dvisc	0.0000578	Pa×s	782.62	Joback Method
dvisc	0.0000434	Pa×s	845.21	Joback Method

Sources

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=U299987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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