5-Bromovaleric acid, hexadecyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-93.66	kJ/mol	Joback Method
hf	-695.24	kJ/mol	Joback Method
hfus	58.22	kJ/mol	Joback Method
hvap	77.93	kJ/mol	Joback Method
log10ws	-7.91		Crippen Method
logp	7.576		Crippen Method
mcvol	331.690	ml/mol	McGowan Method
pc	1027.94	kPa	Joback Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook
tb	822.33	K	Joback Method
tc	1008.86	K	Joback Method
tf	458.39	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.15	J/mol×K	822.33	Joback Method
cpg	1043.09	J/mol×K	853.42	Joback Method
cpg	1061.01	J/mol×K	884.51	Joback Method
cpg	1077.96	J/mol×K	915.59	Joback Method
cpg	1093.96	J/mol×K	946.68	Joback Method
cpg	1109.06	J/mol×K	977.77	Joback Method
cpg	1123.30	J/mol×K	1008.86	Joback Method
dvisc	0.0008628	Pa×s	458.39	Joback Method

dvisc	0.0004077	Pa×s	519.05	Joback Method
dvisc	0.0002253	Pa×s	579.70	Joback Method
dvisc	0.0001394	Pa×s	640.36	Joback Method
dvisc	0.0000937	Pa×s	701.02	Joback Method
dvisc	0.0000671	Pa×s	761.67	Joback Method
dvisc	0.0000504	Pa×s	822.33	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=U292293&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