5-Bromovaleric acid, octadecyl ester

Inchi: InChI=1S/C23H45BrO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-26-23(25)20-17-
InchiKey: BVPJLVJWARICPM-UHFFFAOYSA-N
Formula: C23H45BrO2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCCBr
Mol. weight [g/mol]: 433.51

Physical Properties

Property code	Value	Unit	Source
gf	-76.82	kJ/mol	Joback Method
hf	-736.52	kJ/mol	Joback Method
hfus	63.40	kJ/mol	Joback Method
hvap	82.38	kJ/mol	Joback Method
log10ws	-8.74		Crippen Method
logp	8.356		Crippen Method
mcvol	359.870	ml/mol	McGowan Method
pc	912.18	kPa	Joback Method
rinpol	2824.80		NIST Webbook
tb	868.09	K	Joback Method
tc	1062.80	K	Joback Method
tf	480.93	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1148.37	J/mol×K	868.09	Joback Method
cpg	1237.13	J/mol×K	1030.35	Joback Method
cpg	1221.47	J/mol×K	997.90	Joback Method
cpg	1204.80	J/mol×K	965.45	Joback Method
cpg	1187.10	J/mol×K	932.99	Joback Method
cpg	1168.30	J/mol×K	900.54	Joback Method
cpg	1251.85	J/mol×K	1062.80	Joback Method
dvisc	0.0000373	Pa×s	868.09	Joback Method
dvisc	0.0000498	Pa×s	803.56	Joback Method

dvisc	0.0000699	Pa×s	739.04	Joback Method
dvisc	0.0001049	Pa×s	674.51	Joback Method
dvisc	0.0001713	Pa×s	609.98	Joback Method
dvisc	0.0003143	Pa×s	545.46	Joback Method
dvisc	0.0006785	Pa×s	480.93	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=U292294&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