5-Bromovaleric acid, heptyl ester

Inchi: InChI=1S/C12H23BrO2/c1-2-3-4-5-8-11-15-12(14)9-6-7-10-13/h2-11H2,1H3
InchiKey: NGEGJBIKQPUVST-UHFFFAOYSA-N
Formula: C12H23BrO2
SMILES: CCCCCCCOC(=O)CCCCBr
Mol. weight [g/mol]: 279.21
CAS: 13931-43-6

Physical Properties

Property code	Value	Unit	Source
gf	-169.44	kJ/mol	Joback Method
hf	-509.48	kJ/mol	Joback Method
hfus	34.91	kJ/mol	Joback Method
hvap	57.90	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	4.065		Crippen Method
mcvol	204.880	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	1738.00		NIST Webbook
tb	616.41	K	Joback Method
tc	798.29	K	Joback Method
tf	356.96	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.44	J/mol×K	616.41	Joback Method
cpg	527.35	J/mol×K	646.72	Joback Method
cpg	541.57	J/mol×K	677.04	Joback Method
cpg	555.13	J/mol×K	707.35	Joback Method
cpg	568.03	J/mol×K	737.67	Joback Method
cpg	580.30	J/mol×K	767.98	Joback Method
cpg	591.95	J/mol×K	798.29	Joback Method
dvisc	0.0020531	Pa×s	356.96	Joback Method

dvisc	0.0010894	Pa×s	400.20	Joback Method
dvisc	0.0006541	Pa×s	443.44	Joback Method
dvisc	0.0004300	Pa×s	486.68	Joback Method
dvisc	0.0003027	Pa×s	529.93	Joback Method
dvisc	0.0002247	Pa×s	573.17	Joback Method
dvisc	0.0001739	Pa×s	616.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13931436&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