6-Bromohexanoic acid, 2-methylpentyl ester

Inchi: InChI=1S/C12H23BrO2/c1-3-7-11(2)10-15-12(14)8-5-4-6-9-13/h11H,3-10H2,1-2H3
InchiKey: JMGALUFBIWBQEP-UHFFFAOYSA-N
Formula: C12H23BrO2
SMILES: CCCC(C)COC(=O)CCCCCBr
Mol. weight [g/mol]: 279.21

Physical Properties

Property code	Value	Unit	Source
gf	-171.88	kJ/mol	Joback Method
hf	-514.76	kJ/mol	Joback Method
hfus	31.39	kJ/mol	Joback Method
hvap	57.51	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.921		Crippen Method
mcvol	204.880	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	1737.00		NIST Webbook
tb	615.97	K	Joback Method
tc	800.98	K	Joback Method
tf	341.96	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.85	J/mol×K	615.97	Joback Method
cpg	528.06	J/mol×K	646.81	Joback Method
cpg	542.55	J/mol×K	677.64	Joback Method
cpg	556.34	J/mol×K	708.48	Joback Method
cpg	569.46	J/mol×K	739.31	Joback Method
cpg	581.90	J/mol×K	770.15	Joback Method
cpg	593.71	J/mol×K	800.98	Joback Method
dvisc	0.0025939	Pa×s	341.96	Joback Method
dvisc	0.0012447	Pa×s	387.63	Joback Method

dvisc	0.0006973	Pa×s	433.30	Joback Method
dvisc	0.0004362	Pa×s	478.97	Joback Method
dvisc	0.0002961	Pa×s	524.63	Joback Method
dvisc	0.0002139	Pa×s	570.30	Joback Method
dvisc	0.0001621	Pa×s	615.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354714&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