Hexanoic acid, 3,5,5-trimethyl-, butyl ester

Inchi: InChI=1S/C13H26O2/c1-6-7-8-15-12(14)9-11(2)10-13(3,4)5/h11H,6-10H2,1-5H3
InchiKey: DCWPYGIRDUULGM-UHFFFAOYSA-N
Formula: C13H26O2
SMILES: CCCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]: 214.34

Physical Properties

Property code	Value	Unit	Source
gf	-174.94	kJ/mol	Joback Method
hf	-570.48	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	52.00	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.792		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1746.28	kPa	Joback Method
rinpol	1340.00		NIST Webbook
rinpol	1340.00		NIST Webbook
tb	569.46	K	Joback Method
tc	749.88	K	Joback Method
tf	295.85	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.93	J/mol×K	569.46	Joback Method
cpg	597.48	J/mol×K	719.81	Joback Method
cpg	583.13	J/mol×K	689.74	Joback Method
cpg	568.02	J/mol×K	659.67	Joback Method
cpg	552.13	J/mol×K	629.60	Joback Method
cpg	535.45	J/mol×K	599.53	Joback Method
cpg	611.11	J/mol×K	749.88	Joback Method
dvisc	0.0001454	Pa×s	569.46	Joback Method

dvisc	0.0002029	Pa×s	523.86	Joback Method
dvisc	0.0003018	Pa×s	478.26	Joback Method
dvisc	0.0004881	Pa×s	432.66	Joback Method
dvisc	0.0008840	Pa×s	387.05	Joback Method
dvisc	0.0018762	Pa×s	341.45	Joback Method
dvisc	0.0050223	Pa×s	295.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406054&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

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