Butane-2,3-diol, mono-hexanoate, #1

Inchi: InChI=1S/C12H24O3/c1-6-7-8-9-10(13)15-12(4,5)11(2,3)14/h14H,6-9H2,1-5H3
InchiKey: XGWLGQNKEWAYLA-UHFFFAOYSA-N
Formula: C12H24O3
SMILES: CCCCCC(=O)OC(C)(C)C(C)(C)O
Mol. weight [g/mol]: 216.32

Physical Properties

Property code	Value	Unit	Source
gf	-314.90	kJ/mol	Joback Method
hf	-705.54	kJ/mol	Joback Method
hfus	18.88	kJ/mol	Joback Method
hvap	65.55	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.659		Crippen Method
mcvol	193.250	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	1272.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1272.00		NIST Webbook
tb	635.97	K	Joback Method
tc	816.26	K	Joback Method
tf	362.82	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.03	J/mol×K	635.97	Joback Method
cpg	601.13	J/mol×K	786.21	Joback Method
cpg	589.53	J/mol×K	756.16	Joback Method
cpg	577.25	J/mol×K	726.11	Joback Method
cpg	564.26	J/mol×K	696.07	Joback Method
cpg	550.53	J/mol×K	666.02	Joback Method
cpg	612.11	J/mol×K	816.26	Joback Method

dvisc	0.0000415	Pa×s	635.97	Joback Method
dvisc	0.0000674	Pa×s	590.45	Joback Method
dvisc	0.0001189	Pa×s	544.92	Joback Method
dvisc	0.0002324	Pa×s	499.39	Joback Method
dvisc	0.0005200	Pa×s	453.87	Joback Method
dvisc	0.0013923	Pa×s	408.35	Joback Method
dvisc	0.0047728	Pa×s	362.82	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=R66330&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