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

Inchi: InChI=1S/C10H20O3/c1-6-7-8(11)13-10(4,5)9(2,3)12/h12H,6-7H2,1-5H3
InchiKey: QFBDBBGTTGIOGF-UHFFFAOYSA-N
Formula: C10H20O3
SMILES: CCCC(=O)OC(C)(C)C(C)(C)O
Mol. weight [g/mol]: 188.26

Physical Properties

Property code	Value	Unit	Source
gf	-331.74	kJ/mol	Joback Method
hf	-664.26	kJ/mol	Joback Method
hfus	13.70	kJ/mol	Joback Method
hvap	61.10	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.879		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1076.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1076.00		NIST Webbook
tb	590.21	K	Joback Method
tc	773.51	K	Joback Method
tf	340.28	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.05	J/mol×K	590.21	Joback Method
cpg	495.17	J/mol×K	742.96	Joback Method
cpg	484.49	J/mol×K	712.41	Joback Method
cpg	473.17	J/mol×K	681.86	Joback Method
cpg	461.18	J/mol×K	651.31	Joback Method
cpg	448.48	J/mol×K	620.76	Joback Method
cpg	505.24	J/mol×K	773.51	Joback Method

dvisc	0.0000636	Pa×s	590.21	Joback Method
dvisc	0.0001041	Pa×s	548.56	Joback Method
dvisc	0.0001844	Pa×s	506.90	Joback Method
dvisc	0.0003622	Pa×s	465.25	Joback Method
dvisc	0.0008123	Pa×s	423.59	Joback Method
dvisc	0.0021726	Pa×s	381.94	Joback Method
dvisc	0.0073933	Pa×s	340.28	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=R66312&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