

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

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	1085.00		NIST Webbook
rinpol	1088.00		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/molxK	590.21	Joback Method
cpg	495.17	J/molxK	742.96	Joback Method
cpg	484.49	J/molxK	712.41	Joback Method
cpg	473.17	J/molxK	681.86	Joback Method
cpg	461.18	J/molxK	651.31	Joback Method
cpg	448.48	J/molxK	620.76	Joback Method
cpg	505.24	J/molxK	773.51	Joback Method
dvisc	0.0000636	Paxs	590.21	Joback Method

dvisc	0.0001041	Paxs	548.56	Joback Method
dvisc	0.0001844	Paxs	506.90	Joback Method
dvisc	0.0003622	Paxs	465.25	Joback Method
dvisc	0.0008123	Paxs	423.59	Joback Method
dvisc	0.0021726	Paxs	381.94	Joback Method
dvisc	0.0073933	Paxs	340.28	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R66326&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

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