

hexyl 3-hydroxybutanoate

Inchi:	InChI=1S/C10H20O3/c1-3-4-5-6-7-13-10(12)8-9(2)11/h9,11H,3-8H2,1-2H3
InchiKey:	NUOMIZNYSYMUJI-UHFFFAOYSA-N
Formula:	C10H20O3
SMILES:	CCCCCCOC(=O)CC(C)O
Mol. weight [g/mol]:	188.26

Physical Properties

Property code	Value	Unit	Source
gf	-339.86	kJ/mol	Joback Method
hf	-652.04	kJ/mol	Joback Method
hfus	25.01	kJ/mol	Joback Method
hvap	63.30	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.881		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
ripol	1906.00		NIST Webbook
tb	596.23	K	Joback Method
tc	765.82	K	Joback Method
tf	320.44	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.91	J/molxK	596.23	Joback Method
cpg	486.60	J/molxK	737.56	Joback Method
cpg	476.07	J/molxK	709.29	Joback Method
cpg	465.05	J/molxK	681.03	Joback Method
cpg	453.52	J/molxK	652.76	Joback Method
cpg	441.47	J/molxK	624.50	Joback Method
cpg	496.65	J/molxK	765.82	Joback Method
dvisc	0.0000721	Paxs	596.23	Joback Method
dvisc	0.0001158	Paxs	550.27	Joback Method

dvisc	0.0002026	Paxs	504.30	Joback Method
dvisc	0.0003966	Paxs	458.34	Joback Method
dvisc	0.0009018	Paxs	412.37	Joback Method
dvisc	0.0025198	Paxs	366.41	Joback Method
dvisc	0.0094549	Paxs	320.44	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=R327272&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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