

Hexyl 3-hydroxyhexanoate

Inchi:	InChI=1S/C12H24O3/c1-3-5-6-7-9-15-12(14)10-11(13)8-4-2/h11,13H,3-10H2,1-2H3
InchiKey:	ZRTLWXWZDCVYMO-UHFFFAOYSA-N
Formula:	C12H24O3
SMILES:	CCCCCOC(=O)CC(O)CCC
Mol. weight [g/mol]:	216.32

Physical Properties

Property code	Value	Unit	Source
gf	-323.02	kJ/mol	Joback Method
hf	-693.32	kJ/mol	Joback Method
hfus	30.19	kJ/mol	Joback Method
hvap	67.75	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.661		Crippen Method
mvol	193.250	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
ripol	2066.00		NIST Webbook
ripol	2066.00		NIST Webbook
tb	641.99	K	Joback Method
tc	810.69	K	Joback Method
tf	342.98	K	Joback Method
vc	0.745	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.60	J/molxK	641.99	Joback Method
cpg	544.46	J/molxK	670.11	Joback Method
cpg	557.72	J/molxK	698.22	Joback Method
cpg	570.39	J/molxK	726.34	Joback Method
cpg	582.49	J/molxK	754.46	Joback Method
cpg	594.01	J/molxK	782.57	Joback Method
cpg	604.99	J/molxK	810.69	Joback Method
dvisc	0.0063203	Paxs	342.98	Joback Method

dvisc	0.0016900	Paxs	392.81	Joback Method
dvisc	0.0006081	Paxs	442.65	Joback Method
dvisc	0.0002691	Paxs	492.49	Joback Method
dvisc	0.0001384	Paxs	542.32	Joback Method
dvisc	0.0000796	Paxs	592.15	Joback Method
dvisc	0.0000498	Paxs	641.99	Joback Method

Sources

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=R327287&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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