

12-Hydroxydodecanoic acid

Other names:	Dodecanoic acid, 12-hydroxy-
Inchi:	InChI=1S/C12H24O3/c13-11-9-7-5-3-1-2-4-6-8-10-12(14)15/h13H,1-11H2,(H,14,15)
InchiKey:	ZDHCZVWCTKTBRY-UHFFFAOYSA-N
Formula:	C12H24O3
SMILES:	O=C(O)CCCCCCCCCCCCO
Mol. weight [g/mol]:	216.32
CAS:	505-95-3

Physical Properties

Property code	Value	Unit	Source
gf	-352.40	kJ/mol	Joback Method
hf	-708.05	kJ/mol	Joback Method
hfs	-959.00 ± 3.00	kJ/mol	NIST Webbook
hfus	36.61	kJ/mol	Joback Method
hvap	82.41	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.964		Crippen Method
mcvol	193.250	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
tb	712.19	K	Joback Method
tc	880.34	K	Joback Method
tf	357.00 ± 4.00	K	NIST Webbook
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.97	J/mol×K	712.19	Joback Method
cpg	576.14	J/mol×K	740.22	Joback Method
cpg	587.74	J/mol×K	768.24	Joback Method
cpg	598.81	J/mol×K	796.27	Joback Method
cpg	609.35	J/mol×K	824.29	Joback Method
cpg	619.40	J/mol×K	852.32	Joback Method
cpg	628.96	J/mol×K	880.34	Joback Method

dvisc	0.0038755	Paxs	396.57	Joback Method
dvisc	0.0008530	Paxs	449.17	Joback Method
dvisc	0.0002579	Paxs	501.78	Joback Method
dvisc	0.0000978	Paxs	554.38	Joback Method
dvisc	0.0000439	Paxs	606.98	Joback Method
dvisc	0.0000224	Paxs	659.59	Joback Method
dvisc	0.0000126	Paxs	712.19	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=C505953&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
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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