

Dodecanoic acid, 3-hydroxy-, ethyl ester

Other names:	Ethyl 3-hydroxy dodecanoate
Inchi:	InChI=1S/C14H28O3/c1-3-5-6-7-8-9-10-11-13(15)12-14(16)17-4-2/h13,15H,3-12H2,1-2H1
InchiKey:	CQLRIUYMQWJYSR-UHFFFAOYSA-N
Formula:	C14H28O3
SMILES:	CCCCCCCCCCC(O)CC(=O)OCC
Mol. weight [g/mol]:	244.37
CAS:	126679-28-5

Physical Properties

Property code	Value	Unit	Source
gf	-306.18	kJ/mol	Joback Method
hf	-734.60	kJ/mol	Joback Method
hfus	35.37	kJ/mol	Joback Method
hvap	72.20	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.441		Crippen Method
mcvol	221.430	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	1743.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1743.00		NIST Webbook
tb	687.75	K	Joback Method
tc	857.11	K	Joback Method
tf	365.52	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.98	J/mol×K	687.75	Joback Method
cpg	652.97	J/mol×K	715.98	Joback Method
cpg	667.27	J/mol×K	744.20	Joback Method
cpg	680.92	J/mol×K	772.43	Joback Method
cpg	693.91	J/mol×K	800.66	Joback Method

cpg	706.27	J/mol×K	828.88	Joback Method
cpg	718.00	J/mol×K	857.11	Joback Method
dvisc	0.0042282	Pa×s	365.52	Joback Method
dvisc	0.0011342	Pa×s	419.22	Joback Method
dvisc	0.0004102	Pa×s	472.93	Joback Method
dvisc	0.0001826	Pa×s	526.63	Joback Method
dvisc	0.0000944	Pa×s	580.34	Joback Method
dvisc	0.0000546	Pa×s	634.05	Joback Method
dvisc	0.0000344	Pa×s	687.75	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=C126679285&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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