

Dodecanoic acid, 12-hydroxy-, methyl ester

Inchi:	InChI=1S/C13H26O3/c1-16-13(15)11-9-7-5-3-2-4-6-8-10-12-14/h14H,2-12H2,1H3
InchiKey:	WVYBBOXJKXXXOY-UHFFFAOYSA-N
Formula:	C13H26O3
SMILES:	COC(=O)CCCCCCCCCCCCO
Mol. weight [g/mol]:	230.34
CAS:	71655-36-2

Physical Properties

Property code	Value	Unit	Source
gf	-312.16	kJ/mol	Joback Method
hf	-708.68	kJ/mol	Joback Method
hfus	36.30	kJ/mol	Joback Method
hvap	70.37	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.053		Crippen Method
mcvol	207.340	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
tb	665.31	K	Joback Method
tc	832.17	K	Joback Method
tf	308.00 ± 3.00	K	NIST Webbook
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.17	J/molxK	665.31	Joback Method
cpg	597.40	J/molxK	693.12	Joback Method
cpg	611.03	J/molxK	720.93	Joback Method
cpg	624.05	J/molxK	748.74	Joback Method
cpg	636.47	J/molxK	776.55	Joback Method
cpg	648.32	J/molxK	804.36	Joback Method
cpg	659.59	J/molxK	832.17	Joback Method
dvisc	0.0035060	Paxs	369.25	Joback Method
dvisc	0.0011030	Paxs	418.59	Joback Method

dvisc	0.0004429	Paxs	467.94	Joback Method
dvisc	0.0002116	Paxs	517.28	Joback Method
dvisc	0.0001150	Paxs	566.62	Joback Method
dvisc	0.0000689	Paxs	615.97	Joback Method
dvisc	0.0000446	Paxs	665.31	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=C71655362&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/64-058-7/Dodecanoic-acid-12-hydroxy-methyl-ester.pdf>

Generated by Cheméo on 2024-04-20 05:22:22.431662046 +0000 UTC m=+15879791.352239359.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.