

Dodecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester

Other names:

Laurin, 2-mono-
«beta»-Monolaurin
Glycerol 2-laurate
Lauric acid «beta»-monoglyceride
2-Monolaurin
1,2,3-Propanetriol 2-dodecanoate
Glycerol «beta»-dodecanoate
2-hydroxy-1-(hydroxymethyl)ethyl laurate

Inchi:

InChI=1S/C15H30O4/c1-2-3-4-5-6-7-8-9-10-11-15(18)19-14(12-16)13-17/h14,16-17H,2-

InchiKey:

ZUCMOZYYSZYRRM-UHFFFAOYSA-N

Formula:

C15H30O4

SMILES:

CCCCCCCCCCCC(=O)OC(CO)CO

Mol. weight [g/mol]:

274.40

CAS:

1678-45-1

Physical Properties

Property code	Value	Unit	Source
chs	-9037.50 ± 1.60	kJ/mol	NIST Webbook
gf	-434.58	kJ/mol	Joback Method
hf	-907.47	kJ/mol	Joback Method
hfs	-1152.60 ± 1.90	kJ/mol	NIST Webbook
hfus	42.05	kJ/mol	Joback Method
hvap	91.11	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.804		Crippen Method
mcvol	241.390	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
tb	802.81	K	Joback Method
tc	983.46	K	Joback Method
tf	437.61	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.10	J/mol×K	983.46	Joback Method
cpg	822.58	J/mol×K	953.35	Joback Method
cpg	811.38	J/mol×K	923.24	Joback Method
cpg	799.48	J/mol×K	893.13	Joback Method
cpg	786.86	J/mol×K	863.03	Joback Method
cpg	773.50	J/mol×K	832.92	Joback Method
cpg	759.38	J/mol×K	802.81	Joback Method
cps	436.40	J/mol×K	298.00	NIST Webbook
dvisc	0.0000071	Paxs	741.94	Joback Method
dvisc	0.0000139	Paxs	681.08	Joback Method
dvisc	0.0000311	Paxs	620.21	Joback Method
dvisc	0.0000825	Paxs	559.34	Joback Method
dvisc	0.0002782	Paxs	498.48	Joback Method
dvisc	0.0013156	Paxs	437.61	Joback Method
dvisc	0.0000040	Paxs	802.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1678451&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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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