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

Other names: Decanoin, 2-mono-
Decanoic acid 2-monoglyceride

Inchi: InChI=1S/C13H26O4/c1-2-3-4-5-6-7-8-9-13(16)17-12(10-14)11-15/h12,14-15H,2-11H2,1

InchiKey: IYVVKFYDGRJWTR-UHFFFAOYSA-N

Formula: C13H26O4

SMILES: CCCCCCCCCC(=O)OC(CO)CO

Mol. weight [g/mol]: 246.34

CAS: 3376-48-5

Physical Properties

Property code	Value	Unit	Source
chs	-7735.70 ± 1.90	kJ/mol	NIST Webbook
gf	-451.42	kJ/mol	Joback Method
hf	-866.19	kJ/mol	Joback Method
hfs	-1095.80 ± 2.10	kJ/mol	NIST Webbook
hfus	36.87	kJ/mol	Joback Method
hvap	86.66	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.024		Crippen Method
mcvol	213.210	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
tb	757.05	K	Joback Method
tc	930.94	K	Joback Method
tf	415.07	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.41	J/mol×K	757.05	Joback Method
cpg	659.30	J/mol×K	786.03	Joback Method
cpg	671.55	J/mol×K	815.01	Joback Method
cpg	683.16	J/mol×K	844.00	Joback Method
cpg	694.15	J/mol×K	872.98	Joback Method

cpg	704.54	J/mol×K	901.96	Joback Method
cpg	714.34	J/mol×K	930.94	Joback Method
dvisc	0.0022293	Pa×s	415.07	Joback Method
dvisc	0.0004662	Pa×s	472.07	Joback Method
dvisc	0.0001366	Pa×s	529.06	Joback Method
dvisc	0.0000508	Pa×s	586.06	Joback Method
dvisc	0.0000225	Pa×s	643.06	Joback Method
dvisc	0.0000114	Pa×s	700.05	Joback Method
dvisc	0.0000064	Pa×s	757.05	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3376485&Units=SI
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

Legend

chs: Standard solid enthalpy of combustion
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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