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,3-12H2,1-2H
InchiKey: CQLRIUYMQWJYSR-UHFFFAOYSA-N
Formula: C14H28O3
SMILES: CCCCCCCCCC(O)CC(=O)OCC
Mol. weight [g/mol]: 244.38

Physical Properties

Property code	Value	Unit	Source
af	0.8919		Cheméo Relay (1.0)
gf	-306.18	kJ/mol	Joback Method
hf	-837.77	kJ/mol	Cheméo Relay (1.0)
hfus	35.37	kJ/mol	Joback Method
hvap	90.57	kJ/mol	Cheméo Relay (1.0)
ie	9.82	eV	Cheméo Relay (1.0)
log10ws	-3.50		Cheméo Relay (1.0)
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	558.48	K	Cheméo Relay (1.0)
tc	744.28	K	Cheméo Relay (1.0)
tf	298.57	K	Cheméo Relay (1.0)
vc	0.850	m3/kmol	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C126679285&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
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
ie: Ionization energy
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