TRIDECANOIC ACID, 3-HYDROXY-, ETHYL ESTER

Inchi: InChI=1S/C15H30O3/c1-3-5-6-7-8-9-10-11-12-14(16)13-15(17)18-4-2/h14,16H,3-13H2,1

InchiKey: LOFDGMSAUOHYLH-UHFFFAOYSA-N

Formula: C15H30O3

SMILES: CCCCCCCCCCC(O)CC(=O)OCC

Mol. weight [g/mol]: 258.40

Physical Properties

Property code	Value	Unit	Source
af	0.9271		Cheméo Relay (1.0)
gf	-297.76	kJ/mol	Joback Method
hf	-857.72	kJ/mol	Cheméo Relay (1.0)
hfus	37.96	kJ/mol	Joback Method
hvap	94.96	kJ/mol	Cheméo Relay (1.0)
ie	9.83	eV	Cheméo Relay (1.0)
log10ws	-3.89		Cheméo Relay (1.0)
logp	3.831		Crippen Method
mcvol	235.520	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	1539.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1539.00		NIST Webbook
ripol	2433.00		NIST Webbook
ripol	2433.00		NIST Webbook
tb	571.04	K	Cheméo Relay (1.0)
tc	755.83	K	Cheméo Relay (1.0)
tf	305.30	K	Cheméo Relay (1.0)
vc	0.905	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.58	J/mol×K	710.63	Joback Method
cpg	709.09	J/mol×K	739.03	Joback Method
cpg	723.89	J/mol×K	767.43	Joback Method

cpg	737.97	J/mol×K	795.83	Joback Method
cpg	751.37	J/mol×K	824.23	Joback Method
cpg	764.10	J/mol×K	852.63	Joback Method
cpg	776.17	J/mol×K	881.04	Joback Method
dvisc	0.0034600	Pa×s	376.79	Joback Method
dvisc	0.0009296	Pa×s	432.43	Joback Method
dvisc	0.0003370	Pa×s	488.07	Joback Method
dvisc	0.0001504	Pa×s	543.71	Joback Method
dvisc	0.0000780	Pa×s	599.35	Joback Method
dvisc	0.0000452	Pa×s	654.99	Joback Method
dvisc	0.0000285	Pa×s	710.63	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=C107141151&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
ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume