

2-Hydroxyethyl tridecanoate

Inchi:	InChI=1S/C15H30O3/c1-2-3-4-5-6-7-8-9-10-11-12-15(17)18-14-13-16/h16H,2-14H2,1H3
InchiKey:	FFSGAVLPIGSPIZ-UHFFFAOYSA-N
Formula:	C15H30O3
SMILES:	CCCCCCCCCCCCC(=O)OCCO
Mol. weight [g/mol]:	258.40

Physical Properties

Property code	Value	Unit	Source
gf	-295.32	kJ/mol	Joback Method
hf	-749.96	kJ/mol	Joback Method
hfus	41.48	kJ/mol	Joback Method
hvap	74.82	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.833		Crippen Method
mcvol	235.520	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
rinqol	1914.00		NIST Webbook
tb	711.07	K	Joback Method
tc	880.03	K	Joback Method
tf	391.79	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.10	J/molxK	711.07	Joback Method
cpg	708.46	J/molxK	739.23	Joback Method
cpg	723.11	J/molxK	767.39	Joback Method
cpg	737.09	J/molxK	795.55	Joback Method
cpg	750.39	J/molxK	823.71	Joback Method
cpg	763.03	J/molxK	851.87	Joback Method
cpg	775.04	J/molxK	880.03	Joback Method
dvisc	0.0024295	Paxs	391.79	Joback Method
dvisc	0.0007593	Paxs	445.00	Joback Method

dvisc	0.0003042	Paxs	498.22	Joback Method
dvisc	0.0001454	Paxs	551.43	Joback Method
dvisc	0.0000792	Paxs	604.64	Joback Method
dvisc	0.0000475	Paxs	657.86	Joback Method
dvisc	0.0000308	Paxs	711.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540544&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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

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