OCTANOIC ACID, 2-ETHYLHEXYL ESTER

Other names: 2-Ethylhexyl caprylate
2-ethylhexyl octanoate
Inchi: InChI=1S/C16H32O2/c1-4-7-9-10-11-13-16(17)18-14-15(6-3)12-8-5-2/h15H,4-14H2,1-3H
InchiKey: HPUAIVNIHNEYPO-UHFFFAOYSA-N
Formula: C16H32O2
SMILES: CCCCCCCC(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 256.43

Physical Properties

Property code	Value	Unit	Source
af	0.7790		Cheméo Relay (1.0)
hf	-695.03	kJ/mol	Cheméo Relay (1.0)
hfus	36.46	kJ/mol	Joback Method
hvap	76.04	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.26		Cheméo Relay (1.0)
logp	5.107		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
tb	560.06	K	Cheméo Relay (1.0)
tc	732.61	K	Cheméo Relay (1.0)
tf	206.40	K	Cheméo Relay (1.0)
vc	0.911	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.23	J/mol×K	641.33	Joback Method
cpg	694.40	J/mol×K	669.60	Joback Method
cpg	711.78	J/mol×K	697.86	Joback Method
cpg	728.40	J/mol×K	726.13	Joback Method
cpg	744.26	J/mol×K	754.40	Joback Method
cpg	759.39	J/mol×K	782.67	Joback Method

cpg	773.80	J/mol×K	810.93	Joback Method
dvisc	0.0031617	Pa×s	327.24	Joback Method
dvisc	0.0012389	Pa×s	379.59	Joback Method
dvisc	0.0006092	Pa×s	431.94	Joback Method
dvisc	0.0003493	Pa×s	484.28	Joback Method
dvisc	0.0002232	Pa×s	536.63	Joback Method
dvisc	0.0001544	Pa×s	588.98	Joback Method
dvisc	0.0001135	Pa×s	641.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63321700&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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