Decanoic acid, 2-ethylhexyl ester

Other names: 2-Ethylhexyl caprate
2-ethylhexyl decanoate
Inchi: InChI=1S/C18H36O2/c1-4-7-9-10-11-12-13-15-18(19)20-16-17(6-3)14-8-5-2/h17H,4-16H
InchiKey: XEYIWOWYMLEPSD-UHFFFAOYSA-N
Formula: C18H36O2
SMILES: CCCCCCCCCC(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 284.48
CAS: 73947-30-5

Physical Properties

Property code	Value	Unit	Source
gf	-135.68	kJ/mol	Joback Method
hf	-664.93	kJ/mol	Joback Method
hfus	41.64	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.887		Crippen Method
mcvol	271.920	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook
tb	687.09	K	Joback Method
tc	857.14	K	Joback Method
tf	349.78	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.33	J/mol×K	687.09	Joback Method
cpg	877.02	J/mol×K	828.80	Joback Method
cpg	861.31	J/mol×K	800.46	Joback Method
cpg	844.81	J/mol×K	772.12	Joback Method
cpg	827.49	J/mol×K	743.77	Joback Method

cpg	809.34	J/mol×K	715.43	Joback Method
cpg	891.94	J/mol×K	857.14	Joback Method
dvisc	0.0000883	Pa×s	687.09	Joback Method
dvisc	0.0001207	Pa×s	630.87	Joback Method
dvisc	0.0001755	Pa×s	574.65	Joback Method
dvisc	0.0002766	Pa×s	518.43	Joback Method
dvisc	0.0004870	Pa×s	462.22	Joback Method
dvisc	0.0010029	Pa×s	406.00	Joback Method
dvisc	0.0026053	Pa×s	349.78	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73947305&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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