

2-Heptenoic acid, 2-ethylhexyl ester

Inchi:	InChI=1S/C15H28O2/c1-4-7-9-10-12-15(16)17-13-14(6-3)11-8-5-2/h10,12,14H,4-9,11,13
InchiKey:	VYTXNOZINPENJS-ZRDIBKRKSA-N
Formula:	C15H28O2
SMILES:	CCCCC=CC(=O)OCC(CC)CCCC
Mol. weight [g/mol]:	240.38

Physical Properties

Property code	Value	Unit	Source
gf	-80.72	kJ/mol	Joback Method
hf	-485.79	kJ/mol	Joback Method
hfus	34.07	kJ/mol	Joback Method
hvap	57.71	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.492		Crippen Method
mvol	225.350	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	1678.00		NIST Webbook
rinpol	1678.00		NIST Webbook
tb	622.61	K	Joback Method
tc	798.28	K	Joback Method
tf	310.89	K	Joback Method
vc	0.874	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.96	J/molxK	622.61	Joback Method
cpg	618.28	J/molxK	651.89	Joback Method
cpg	634.82	J/molxK	681.17	Joback Method
cpg	650.60	J/molxK	710.44	Joback Method
cpg	665.65	J/molxK	739.72	Joback Method
cpg	679.98	J/molxK	769.00	Joback Method
cpg	693.62	J/molxK	798.28	Joback Method
dvisc	0.0032461	Paxs	310.89	Joback Method

dvisc	0.0012311	Paxs	362.84	Joback Method
dvisc	0.0005952	Paxs	414.80	Joback Method
dvisc	0.0003383	Paxs	466.75	Joback Method
dvisc	0.0002154	Paxs	518.70	Joback Method
dvisc	0.0001488	Paxs	570.66	Joback Method
dvisc	0.0001094	Paxs	622.61	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406903&Units=SI

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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