Hexanoic acid, 2-ethylhexyl ester

Other names:	2-Ethylhexyl caproate
	2-ethylhexyl hexanoate
Inchi:	InChI=1S/C14H28O2/c1-4-7-9-11-14(15)16-12-13(6-3)10-8-5-2/h13H,4-12H2,1-3H3
InchiKey:	QRNFTMKPBPCPJO-UHFFFAOYSA-N
Formula:	C14H28O2
SMILES:	CCCCCC(=O)OCC(CC)CCCC
Mol. weight [g/mol]:	228.37
CAS:	16397-75-4

Physical Properties

Property code	Value	Unit	Source
gf	-169.36	kJ/mol	Joback Method
hf	-582.37	kJ/mol	Joback Method
hfus	31.28	kJ/mol	Joback Method
hvap	55.53	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.326		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	1497.00		NIST Webbook
tb	595.57	K	Joback Method
tc	766.26	K	Joback Method
tf	304.70	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.35	J/mol×K	595.57	Joback Method
cpg	584.55	J/mol×K	624.02	Joback Method
cpg	601.04	J/mol×K	652.47	Joback Method
cpg	616.82	J/mol×K	680.91	Joback Method
cpg	631.92	J/mol×K	709.36	Joback Method
cpg	646.34	J/mol×K	737.81	Joback Method

cpg	660.10	J/mol×K	766.26	Joback Method
dvisc	0.0037349	Pa×s	304.70	Joback Method
dvisc	0.0014934	Pa×s	353.18	Joback Method
dvisc	0.0007451	Pa×s	401.66	Joback Method
dvisc	0.0004318	Pa×s	450.13	Joback Method
dvisc	0.0002782	Pa×s	498.61	Joback Method
dvisc	0.0001938	Pa×s	547.09	Joback Method
dvisc	0.0001432	Pa×s	595.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16397754&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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