

Octanoic acid, 2-hexenyl ester, (E)-

Other names:	trans-2-Hexenyl n-octanoate (2E)-2-Hexenyl octanoate (E)-2-Hexenyl octanoate
Inchi:	InChI=1S/C14H26O2/c1-3-5-7-9-10-12-14(15)16-13-11-8-6-4-2/h8,11H,3-7,9-10,12-13H2
InchiKey:	IRUGSDVUJNNIMW-DHZHZOJOSA-N
Formula:	C14H26O2
SMILES:	CCCC=CCOC(=O)CCCCCCC
Mol. weight [g/mol]:	226.35
CAS:	85554-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-86.70	kJ/mol	Joback Method
hf	-459.87	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	55.87	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.246		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	1573.00		NIST Webbook
ripol	1853.00		NIST Webbook
tb	600.17	K	Joback Method
tc	774.06	K	Joback Method
tf	314.62	K	Joback Method
vc	0.824	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.45	J/mol×K	600.17	Joback Method
cpg	563.96	J/mol×K	629.15	Joback Method
cpg	579.75	J/mol×K	658.13	Joback Method
cpg	594.83	J/mol×K	687.12	Joback Method

cpg	609.24	J/mol×K	716.10	Joback Method
cpg	622.98	J/mol×K	745.08	Joback Method
cpg	636.08	J/mol×K	774.06	Joback Method
dvisc	0.0025872	Paxs	314.62	Joback Method
dvisc	0.0011349	Paxs	362.21	Joback Method
dvisc	0.0006028	Paxs	409.80	Joback Method
dvisc	0.0003653	Paxs	457.40	Joback Method
dvisc	0.0002432	Paxs	504.99	Joback Method
dvisc	0.0001737	Paxs	552.58	Joback Method
dvisc	0.0001309	Paxs	600.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C85554729&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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