

Octanoic acid, 3-hexenyl ester, (Z)-

Other names:	cis-3-Hexanyl n-octanoate (3Z)-3-Hexenyl octanoate cis-3-hexenyl octanoate (Z)-3-Hexenyl octanoate Octanoic acid, (3Z)-3-hexen-1-yl ester
Inchi:	InChI=1S/C14H26O2/c1-3-5-7-9-10-12-14(15)16-13-11-8-6-4-2/h6,8H,3-5,7,9-13H2,1-2H
InchiKey:	DYIDDAHUMHEEQ-VURMDHGXSA-N
Formula:	C14H26O2
SMILES:	CCC=CCCOC(=O)CCCCCCC
Mol. weight [g/mol]:	226.35
CAS:	61444-41-5

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	1561.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1559.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1837.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1837.00		NIST Webbook
ripol	1837.00		NIST Webbook

ripol	1838.00		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/molxK	600.17	Joback Method
cpg	622.98	J/molxK	745.08	Joback Method
cpg	609.24	J/molxK	716.10	Joback Method
cpg	594.83	J/molxK	687.12	Joback Method
cpg	579.75	J/molxK	658.13	Joback Method
cpg	563.96	J/molxK	629.15	Joback Method
cpg	636.08	J/molxK	774.06	Joback Method
dvisc	0.0001309	Paxs	600.17	Joback Method
dvisc	0.0001737	Paxs	552.58	Joback Method
dvisc	0.0002432	Paxs	504.99	Joback Method
dvisc	0.0003653	Paxs	457.40	Joback Method
dvisc	0.0006028	Paxs	409.80	Joback Method
dvisc	0.0011349	Paxs	362.21	Joback Method
dvisc	0.0025872	Paxs	314.62	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=C61444415&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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