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

Other names: cis-3-Hexenyl n-decanoate
(3Z)-3-Hexenyl decanoate
cis-3-Hexenyl decanoate
(Z)-3-Hexenyl decanoate
Inchi: InChI=1S/C16H30O2/c1-3-5-7-9-10-11-12-14-16(17)18-15-13-8-6-4-2/h6,8H,3-5,7,9-15H
InchiKey: APSRJAGZYONPLL-VURMDHGXSA-N
Formula: C16H30O2
SMILES: CCC=CCCOC(=O)CCCCCCCCC
Mol. weight [g/mol]: 254.41
CAS: 85554-69-4

Physical Properties

Property code	Value	Unit	Source
gf	-69.86	kJ/mol	Joback Method
hf	-501.15	kJ/mol	Joback Method
hfus	40.18	kJ/mol	Joback Method
hvap	60.32	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	5.027		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2038.00		NIST Webbook
tb	645.93	K	Joback Method
tc	818.34	K	Joback Method
tf	337.16	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.12	J/mol×K	645.93	Joback Method

cpg	734.94	J/mol×K	789.61	Joback Method
cpg	720.44	J/mol×K	760.87	Joback Method
cpg	705.23	J/mol×K	732.14	Joback Method
cpg	689.29	J/mol×K	703.40	Joback Method
cpg	672.59	J/mol×K	674.67	Joback Method
cpg	748.76	J/mol×K	818.34	Joback Method
dvisc	0.0001048	Pa×s	645.93	Joback Method
dvisc	0.0001400	Pa×s	594.47	Joback Method
dvisc	0.0001976	Pa×s	543.01	Joback Method
dvisc	0.0002997	Pa×s	491.55	Joback Method
dvisc	0.0005012	Pa×s	440.08	Joback Method
dvisc	0.0009605	Pa×s	388.62	Joback Method
dvisc	0.0022449	Pa×s	337.16	Joback Method

Sources

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=C85554694&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume