

Hexanoic acid, 1-ethenyl-1,5-dimethyl-4-hexenyl ester

Other names:

Linalyl n-hexanoate

1,5-Dimethyl-1-vinyl-4-hexenyl hexanoate

Linalyl hexanoate

Linalyl caproate

1,5-dimethyl-1-vinylhex-4-enyl hexanoate

Inchi: InChI=1S/C16H28O2/c1-6-8-9-12-15(17)18-16(5,7-2)13-10-11-14(3)4/h7,11H,2,6,8-10,1

InchiKey: ALKCLFLTxBBMMP-UHFFFAOYSA-N

Formula: C16H28O2

SMILES: C=CC(C)(CCC=C(C)C)OC(=O)CCCCC

Mol. weight [g/mol]: 252.39

CAS: 7779-23-9

Physical Properties

Property code	Value	Unit	Source
gf	12.27	kJ/mol	Joback Method
hf	-394.26	kJ/mol	Joback Method
hfus	30.18	kJ/mol	Joback Method
hvap	58.44	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.801		Crippen Method
mcvol	235.140	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
ripol	1582.00		NIST Webbook
ripol	1844.00		NIST Webbook
ripol	1844.00		NIST Webbook
ripol	1843.00		NIST Webbook
tb	639.26	K	Joback Method
tc	823.96	K	Joback Method
tf	323.86	K	Joback Method
vc	0.906	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	634.68	J/mol×K	639.26	Joback Method
cpg	652.49	J/mol×K	670.04	Joback Method
cpg	669.37	J/mol×K	700.83	Joback Method
cpg	685.38	J/mol×K	731.61	Joback Method
cpg	700.55	J/mol×K	762.39	Joback Method
cpg	714.93	J/mol×K	793.18	Joback Method
cpg	728.57	J/mol×K	823.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7779239&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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

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