

3-Octenoic acid, 4-methyl-2-pentyl ester

Inchi:	InChI=1S/C14H26O2/c1-5-6-7-8-9-10-14(15)16-13(4)11-12(2)3/h8-9,12-13H,5-7,10-11H2
InchiKey:	HCTGXNACTPGUST-CMDGGGOBGSA-N
Formula:	C14H26O2
SMILES:	CCCCC=CCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]:	226.35

Physical Properties

Property code	Value	Unit	Source
gf	-91.58	kJ/mol	Joback Method
hf	-470.43	kJ/mol	Joback Method
hfus	27.96	kJ/mol	Joback Method
hvap	55.10	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	4.101		Crippen Method
mvol	211.260	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	1491.00		NIST Webbook
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tb	599.29	K	Joback Method
tc	779.11	K	Joback Method
tf	284.62	K	Joback Method
vc	0.811	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.16	J/molxK	599.29	Joback Method
cpg	565.33	J/molxK	629.26	Joback Method
cpg	581.71	J/molxK	659.23	Joback Method
cpg	597.32	J/molxK	689.20	Joback Method
cpg	612.19	J/molxK	719.17	Joback Method
cpg	626.35	J/molxK	749.14	Joback Method
cpg	639.81	J/molxK	779.11	Joback Method
dvisc	0.0049998	Paxs	284.62	Joback Method

dvisc	0.0016313	Paxs	337.06	Joback Method
dvisc	0.0007196	Paxs	389.51	Joback Method
dvisc	0.0003855	Paxs	441.95	Joback Method
dvisc	0.0002357	Paxs	494.40	Joback Method
dvisc	0.0001584	Paxs	546.85	Joback Method
dvisc	0.0001141	Paxs	599.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406126&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
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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