

2-Heptenoic acid, 4-methyl-2-pentyl ester

Inchi:	InChI=1S/C13H24O2/c1-5-6-7-8-9-13(14)15-12(4)10-11(2)3/h8-9,11-12H,5-7,10H2,1-4H
InchiKey:	JPSUTLBTGVSEDA-CMDGGOBGSA-N
Formula:	C13H24O2
SMILES:	CCCCC=CC(=O)OC(C)CC(C)C
Mol. weight [g/mol]:	212.33

Physical Properties

Property code	Value	Unit	Source
gf	-100.00	kJ/mol	Joback Method
hf	-449.79	kJ/mol	Joback Method
hfus	25.37	kJ/mol	Joback Method
hvap	52.87	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.711		Crippen Method
mvol	197.170	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	1413.00		NIST Webbook
rinpol	1413.00		NIST Webbook
tb	576.41	K	Joback Method
tc	757.85	K	Joback Method
tf	273.35	K	Joback Method
vc	0.755	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.46	J/molxK	576.41	Joback Method
cpg	572.25	J/molxK	727.61	Joback Method
cpg	558.53	J/molxK	697.37	Joback Method
cpg	544.10	J/molxK	667.13	Joback Method
cpg	528.96	J/molxK	636.89	Joback Method
cpg	513.09	J/molxK	606.65	Joback Method
cpg	585.30	J/molxK	757.85	Joback Method
dvisc	0.0001271	Paxs	576.41	Joback Method

dvisc	0.0001760	Paxs	525.90	Joback Method
dvisc	0.0002612	Paxs	475.39	Joback Method
dvisc	0.0004259	Paxs	424.88	Joback Method
dvisc	0.0007923	Paxs	374.37	Joback Method
dvisc	0.0017887	Paxs	323.86	Joback Method
dvisc	0.0054561	Paxs	273.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U406091&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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