

2-methyl-5-phenyl-2-hexenal

Inchi:	InChI=1S/C13H18O/c1-11(10-14)8-9-12(2)13-6-4-3-5-7-13/h3-7,10-12H,8-9H2,1-2H3
InchiKey:	QPASYBVRNDPIRI-UHFFFAOYSA-N
Formula:	C13H18O
SMILES:	CC(C=O)CCC(C)c1ccccc1
Mol. weight [g/mol]:	190.28

Physical Properties

Property code	Value	Unit	Source
gf	66.59	kJ/mol	Joback Method
hf	-171.26	kJ/mol	Joback Method
hfus	18.71	kJ/mol	Joback Method
hvap	52.75	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.405		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
ripol	2029.00		NIST Webbook
ripol	2029.00		NIST Webbook
tb	571.30	K	Joback Method
tc	780.02	K	Joback Method
tf	274.69	K	Joback Method
vc	0.660	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.95	J/molxK	571.30	Joback Method
cpg	434.58	J/molxK	606.09	Joback Method
cpg	450.21	J/molxK	640.87	Joback Method
cpg	464.89	J/molxK	675.66	Joback Method
cpg	478.65	J/molxK	710.45	Joback Method
cpg	491.55	J/molxK	745.23	Joback Method
cpg	503.61	J/molxK	780.02	Joback Method
dvisc	0.0064620	Paxs	274.69	Joback Method

dvisc	0.0023313	Paxs	324.12	Joback Method
dvisc	0.0011016	Paxs	373.56	Joback Method
dvisc	0.0006202	Paxs	423.00	Joback Method
dvisc	0.0003938	Paxs	472.43	Joback Method
dvisc	0.0002725	Paxs	521.87	Joback Method
dvisc	0.0002010	Paxs	571.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R312275&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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