

5-Methyl-1-phenyl-1-hexen-3-one, trans

Inchi:	InChI=1S/C13H16O/c1-11(2)10-13(14)9-8-12-6-4-3-5-7-12/h3-9,11H,10H2,1-2H3/b9-8+
InchiKey:	LLVCDRTZBYXKII-CMDGGOBGSA-N
Formula:	C13H16O
SMILES:	CC(C)CC(=O)C=Cc1ccccc1
Mol. weight [g/mol]:	188.27
CAS:	60796-12-5

Physical Properties

Property code	Value	Unit	Source
gf	119.85	kJ/mol	Joback Method
hf	-75.76	kJ/mol	Joback Method
hfus	21.75	kJ/mol	Joback Method
hvap	53.12	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.315		Crippen Method
mcvol	167.540	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
tb	581.11	K	Joback Method
tc	799.47	K	Joback Method
tf	292.54	K	Joback Method
vc	0.635	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.71	J/mol×K	581.11	Joback Method
cpg	413.81	J/mol×K	617.50	Joback Method
cpg	428.85	J/mol×K	653.90	Joback Method
cpg	442.90	J/mol×K	690.29	Joback Method
cpg	456.00	J/mol×K	726.69	Joback Method
cpg	468.22	J/mol×K	763.08	Joback Method
cpg	479.63	J/mol×K	799.47	Joback Method
dvisc	0.0037099	Paxs	292.54	Joback Method
dvisc	0.0015352	Paxs	340.63	Joback Method

dvisc	0.0007903	Paxs	388.73	Joback Method
dvisc	0.0004709	Paxs	436.83	Joback Method
dvisc	0.0003109	Paxs	484.92	Joback Method
dvisc	0.0002212	Paxs	533.01	Joback Method
dvisc	0.0001666	Paxs	581.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60796125&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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