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	m3/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	Pa×s	292.54	Joback Method
dvisc	0.0015352	Pa×s	340.63	Joback Method

dvisc	0.0007903	Pa×s	388.73	Joback Method
dvisc	0.0004709	Pa×s	436.83	Joback Method
dvisc	0.0003109	Pa×s	484.92	Joback Method
dvisc	0.0002212	Pa×s	533.01	Joback Method
dvisc	0.0001666	Pa×s	581.11	Joback Method

Sources

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=C60796125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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