3,5-hexadien-2-one

Other names: hexa-3,5-dien-2-one
Inchi: InChI=1S/C6H8O/c1-3-4-5-6(2)7/h3-5H,1H2,2H3/b5-4+
InchiKey: DACOGBAZMZEGQL-SNAWJCMRSA-N
Formula: C6H8O
SMILES: C=CC=CC(C)=O
Mol. weight [g/mol]: 96.13
CAS: 2957-06-4

Physical Properties

Property code	Value	Unit	Source
gf	38.78	kJ/mol	Joback Method
hf	-37.10	kJ/mol	Joback Method
hfus	11.82	kJ/mol	Joback Method
hvap	34.98	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.318		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
rinpol	811.00		NIST Webbook
rinpol	811.00		NIST Webbook
tb	391.39	K	Joback Method
tc	582.34	K	Joback Method
tf	200.47	K	Joback Method
vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.37	J/mol×K	391.39	Joback Method
cpg	157.45	J/mol×K	423.21	Joback Method
cpg	166.04	J/mol×K	455.04	Joback Method
cpg	174.16	J/mol×K	486.86	Joback Method
cpg	181.83	J/mol×K	518.69	Joback Method
cpg	189.07	J/mol×K	550.51	Joback Method

cpg	195.91	J/mol×K	582.34	Joback Method
dvisc	0.0029704	Pa×s	200.47	Joback Method
dvisc	0.0014668	Pa×s	232.29	Joback Method
dvisc	0.0008585	Pa×s	264.11	Joback Method
dvisc	0.0005638	Pa×s	295.93	Joback Method
dvisc	0.0004018	Pa×s	327.75	Joback Method
dvisc	0.0003040	Pa×s	359.57	Joback Method
dvisc	0.0002407	Pa×s	391.39	Joback Method

Sources

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=C2957064&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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