3,5-Heptadien-2-one, 6-methyl-, (E)-

Other names:	(3E)-6-Methyl-3,5-heptadien-2-one
	6-methyl-(E)-3,5-heptadien-2-one
	(E)-6-methyl-3,5-heptadien-2-one
	(E)-6-Methyl-3,5-heptadienone
	(E)-6-methylhepta-3,5-dien-2-one
	6-Methyl-trans-3,5-heptadien-2-one
Inchi:	InChI=1S/C8H12O/c1-7(2)5-4-6-8(3)9/h4-6H,1-3H3/b6-4+
InchiKey:	KSKXSFZGARKWOW-GQCTYLIASA-N
Formula:	C8H12O
SMILES:	CC(=O)C=CC=C(C)C
Mol. weight [g/mol]:	124.18
CAS:	16647-04-4

Physical Properties

Property code	Value	Unit	Source
gf	39.45	kJ/mol	Joback Method
hf	-96.38	kJ/mol	Joback Method
hfus	17.17	kJ/mol	Joback Method
hvap	40.14	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.098		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1107.40		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1074.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1575.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1561.00		NIST Webbook
tb	444.51	K	Joback Method
tc	641.39	K	Joback Method
tf	205.73	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.66	J/mol×K	444.51	Joback Method
cpg	235.68	J/mol×K	477.32	Joback Method
cpg	247.03	J/mol×K	510.14	Joback Method
cpg	257.73	J/mol×K	542.95	Joback Method
cpg	267.82	J/mol×K	575.76	Joback Method
cpg	277.33	J/mol×K	608.58	Joback Method
cpg	286.31	J/mol×K	641.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16647044&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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