6-Methyl-3,5-heptadiene-2-one

Other names:	6-Methyl-3,5-heptadien-2-one
	6-Methyl-3,5-heptadienone-2
	3,5-Heptadien-2-one, 6-methyl-
	2-methyl-2,4-heptadien-6-one
	6-Methylhepta-3,5-dien-2-one
	6-Methyl-hepta-3,5-diene-2-one
Inchi:	InChI=1S/C8H12O/c1-7(2)5-4-6-8(3)9/h4-6H,1-3H3
InchiKey:	KSKXSFZGARKWOW-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	CC(=O)C=CC=C(C)C
Mol. weight [g/mol]:	124.18
CAS:	1604-28-0

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	1086.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1074.90		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1110.00		NIST Webbook

rinpol	1088.00		NIST Webbook
rinpol	1074.90		NIST Webbook
rinpol	1074.90		NIST Webbook
rinpol	1106.90		NIST Webbook
rinpol	1106.50		NIST Webbook
rinpol	1106.30		NIST Webbook
rinpol	1107.30		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1107.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1604.00		NIST Webbook
ripol	1604.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1602.00		NIST Webbook
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ripol	1602.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1604.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1590.00		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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.50 ± 0.50	K	2.70	NIST Webbook

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=C1604280&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume