2-Cyclopenten-1-one, 3,4,5-trimethyl-

Other names: 3,4,5-Trimethyl-2-cyclopenten-1-one
Inchi: InChI=1S/C8H12O/c1-5-4-8(9)7(3)6(5)2/h4,6-7H,1-3H3
InchiKey: LPBXNOSWWUFYQN-UHFFFAOYSA-N
Formula: C8H12O
SMILES: CC1=CC(=O)C(C)C1C
Mol. weight [g/mol]: 124.18
CAS: 55683-21-1

Physical Properties

Property code	Value	Unit	Source
gf	-56.94	kJ/mol	Joback Method
hf	-259.70	kJ/mol	Joback Method
hfus	11.82	kJ/mol	Joback Method
hvap	38.55	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.788		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
rinpol	1063.00		NIST Webbook
rinpol	1063.00		NIST Webbook
ripol	1483.00		NIST Webbook
tb	465.01	K	Joback Method
tc	680.18	K	Joback Method
tf	268.08	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.35	J/mol×K	465.01	Joback Method
cpg	247.85	J/mol×K	500.87	Joback Method
cpg	261.78	J/mol×K	536.73	Joback Method
cpg	275.15	J/mol×K	572.60	Joback Method
cpg	287.93	J/mol×K	608.46	Joback Method

cpg	300.13	J/mol×K	644.32	Joback Method
cpg	311.72	J/mol×K	680.18	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55683211&Units=SI

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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