CYCLOPENTANONE, 2,3-DIMETHYL-

Inchi: InChI=1S/C7H12O/c1-5-3-4-7(8)6(5)2/h5-6H,3-4H2,1-2H3
InchiKey: NHHSVMBOTBXSFH-UHFFFAOYSA-N
Formula: C7H12O
SMILES: CC1CCC(=O)C1C
Mol. weight [g/mol]: 112.17

Physical Properties

Property code	Value	Unit	Source
hfus	8.40	kJ/mol	Joback Method
hvap	43.92	kJ/mol	Cheméo Relay (1.0)
ie	9.25	eV	Cheméo Relay (1.0)
log10ws	-1.24		Cheméo Relay (1.0)
logp	1.621		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
rinpol	787.00		NIST Webbook
tb	419.69	K	Cheméo Relay (1.0)
tf	289.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.74	J/mol×K	437.99	Joback Method
cpg	220.71	J/mol×K	473.74	Joback Method
cpg	235.09	J/mol×K	509.49	Joback Method
cpg	248.89	J/mol×K	545.24	Joback Method
cpg	262.09	J/mol×K	580.99	Joback Method
cpg	274.68	J/mol×K	616.74	Joback Method
cpg	286.66	J/mol×K	652.49	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U151067&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point