2-ACETONYLCYCLOHEXANONE

Inchi: InChI=1S/C9H14O2/c1-7(10)6-8-4-2-3-5-9(8)11/h8H,2-6H2,1H3
InchiKey: ZBEKDHUCMTXKAO-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CC(=O)CC1CCCCC1=O
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
hfus	12.01	kJ/mol	Joback Method
hvap	61.38	kJ/mol	Cheméo Relay (1.0)
ie	9.18	eV	Cheméo Relay (1.0)
log10ws	-0.98		Cheméo Relay (1.0)
logp	1.725		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
rinpol	1354.00		NIST Webbook
tb	509.36	K	Cheméo Relay (1.0)
tf	307.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.16	J/mol×K	546.56	Joback Method
cpg	331.03	J/mol×K	584.25	Joback Method
cpg	347.01	J/mol×K	621.95	Joback Method
cpg	362.09	J/mol×K	659.64	Joback Method
cpg	376.28	J/mol×K	697.34	Joback Method
cpg	389.55	J/mol×K	735.03	Joback Method
cpg	401.92	J/mol×K	772.73	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=C6126530&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