trans-3,4-Dimethylcyclopentanone

Inchi: InChI=1S/C7H12O/c1-5-3-7(8)4-6(5)2/h5-6H,3-4H2,1-2H3/t5-,6-/m0/s1
InchiKey: ZMGMYCHEWPVBEL-WDSKDSINSA-N
Formula: C7H12O
SMILES: CC1CC(=O)CC1C
Mol. weight [g/mol]: 112.17
CAS: 19550-73-3

Physical Properties

Property code	Value	Unit	Source
gf	-85.69	kJ/mol	Joback Method
hf	-285.37	kJ/mol	Joback Method
hfus	8.40	kJ/mol	Joback Method
hvap	35.37	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.621		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
tb	437.99	K	Joback Method
tc	652.49	K	Joback Method
tf	243.53	K	Joback Method
vc	0.374	m3/kmol	Joback Method

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:	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=C19550733&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume