2,3-dimethyl-4-isopropyl-1-cyclopentanone

Inchi: InChI=1S/C10H18O/c1-6(2)9-5-10(11)8(4)7(9)3/h6-9H,5H2,1-4H3
InchiKey: GYOSSKZVOVKLGG-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CC(C)C1CC(=O)C(C)C1C
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-70.58	kJ/mol	Joback Method
hf	-372.91	kJ/mol	Joback Method
hfus	13.72	kJ/mol	Joback Method
hvap	41.35	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.504		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1126.00		NIST Webbook
tb	501.52	K	Joback Method
tc	711.60	K	Joback Method
tf	258.10	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.05	J/mol×K	501.52	Joback Method
cpg	358.12	J/mol×K	536.53	Joback Method
cpg	376.38	J/mol×K	571.55	Joback Method
cpg	393.81	J/mol×K	606.56	Joback Method
cpg	410.42	J/mol×K	641.57	Joback Method
cpg	426.19	J/mol×K	676.58	Joback Method
cpg	441.13	J/mol×K	711.60	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=R187509&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume