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

Inchi: InChI=1S/C10H16O/c1-6(2)9-5-10(11)8(4)7(9)3/h7-9H,1,5H2,2-4H3
InchiKey: CZUYJUUMDUMIDE-UHFFFAOYSA-N
Formula: C10H16O
SMILES: C=C(C)C1CC(=O)C(C)C1C
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	11.15	kJ/mol	Joback Method
hf	-251.99	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	41.15	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.424		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1113.00		NIST Webbook
tb	498.52	K	Joback Method
tc	712.47	K	Joback Method
tf	257.38	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.38	J/mol×K	498.52	Joback Method
cpg	338.69	J/mol×K	534.18	Joback Method
cpg	356.18	J/mol×K	569.84	Joback Method
cpg	372.84	J/mol×K	605.50	Joback Method
cpg	388.69	J/mol×K	641.15	Joback Method
cpg	403.71	J/mol×K	676.81	Joback Method
cpg	417.91	J/mol×K	712.47	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=R187490&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