7,7-Dimethylbicyclo[3.3.0]octan-2-one

Other names: 7,7-Dimethylbicyclo[3.3.0]-octane-2-one
Inchi: InChI=1S/C10H16O/c1-10(2)5-7-3-4-9(11)8(7)6-10/h7-8H,3-6H2,1-2H3
InchiKey: HTCXXOQBBXKJIN-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1(C)CC2CCC(=O)C2C1
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	-5.17	kJ/mol	Joback Method
hf	-259.25	kJ/mol	Joback Method
hfus	8.01	kJ/mol	Joback Method
hvap	40.81	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.402		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	1378.00		NIST Webbook
rinpol	1376.00		NIST Webbook
tb	513.61	K	Joback Method
tc	745.29	K	Joback Method
tf	319.18	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.59	J/mol×K	513.61	Joback Method
cpg	344.04	J/mol×K	552.22	Joback Method
cpg	362.21	J/mol×K	590.84	Joback Method
cpg	379.23	J/mol×K	629.45	Joback Method
cpg	395.23	J/mol×K	668.06	Joback Method
cpg	410.36	J/mol×K	706.68	Joback Method
cpg	424.76	J/mol×K	745.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R287382&Units=SI
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

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