1s,2r,5r-3-Pinanone

Inchi: InChI=1S/C11H18O/c1-7-9-5-4-8(6-10(7)12)11(9,2)3/h7-9H,4-6H2,1-3H3/t7-,8+,9+/m1/s1
InchiKey: ABXBNWJKXXCADH-VGMNWLOBSA-N
Formula: C10H16O
SMILES: CC1C(=O)CC2CCC1C2(C)C
Mol. weight [g/mol]: 152.23
CAS: 22339-21-5

Physical Properties

Property code	Value	Unit	Source
gf	-4.46	kJ/mol	Joback Method
hf	-153.00 ± 8.40	kJ/mol	NIST Webbook
hfus	11.67	kJ/mol	Joback Method
hvap	42.73	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.648		Crippen Method
mcvol	145.700	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
tb	531.82	K	Joback Method
tc	759.17	K	Joback Method
tf	326.21	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.23	J/mol×K	531.82	Joback Method
cpg	393.80	J/mol×K	569.71	Joback Method
cpg	413.11	J/mol×K	607.60	Joback Method
cpg	431.29	J/mol×K	645.50	Joback Method
cpg	448.46	J/mol×K	683.39	Joback Method
cpg	464.75	J/mol×K	721.28	Joback Method
cpg	480.28	J/mol×K	759.17	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=C22339215&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume