Bicyclo[2.4.0]octan-2-one, 3,3-dimethyl-5-oxa-

Inchi: InChI=1S/C9H14O2/c1-9(2)7(10)6-4-3-5-11-8(6)9/h6,8H,3-5H2,1-2H3
InchiKey: KLTAJTHKXFNMDQ-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CC1(C)C(=O)C2CCCOC21
Mol. weight [g/mol]: 154.21
CAS: 7176-96-7

Physical Properties

Property code	Value	Unit	Source
gf	-99.71	kJ/mol	Joback Method
hf	-370.61	kJ/mol	Joback Method
hfus	13.40	kJ/mol	Joback Method
hvap	43.09	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.390		Crippen Method
mcvol	123.390	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
tb	517.68	K	Joback Method
tc	751.35	K	Joback Method
tf	334.48	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.65	J/mol×K	517.68	Joback Method
cpg	327.47	J/mol×K	556.62	Joback Method
cpg	344.09	J/mol×K	595.57	Joback Method
cpg	359.66	J/mol×K	634.51	Joback Method
cpg	374.31	J/mol×K	673.46	Joback Method
cpg	388.17	J/mol×K	712.40	Joback Method
cpg	401.38	J/mol×K	751.35	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=C7176967&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