7-Oxabicyclo[2.2.1]heptanone, 3,5,6-trimethylidene-

Inchi: InChI=1S/C9H8O2/c1-4-5(2)9-7(10)6(3)8(4)11-9/h8-9H,1-3H2
InchiKey: HLQGJHVUXDBZQM-UHFFFAOYSA-N
Formula: C9H8O2
SMILES: C=C1C(=C)C2OC1C(=C)C2=O
Mol. weight [g/mol]: 148.16
CAS: 127750-96-3

Physical Properties

Property code	Value	Unit	Source
gf	84.83	kJ/mol	Joback Method
hf	-106.63	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	44.86	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-1.53		Crippen Method
logp	1.005		Crippen Method
mcvol	110.490	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
tb	515.32	K	Joback Method
tc	737.13	K	Joback Method
tf	359.38	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.31	J/mol×K	515.32	Joback Method
cpg	266.44	J/mol×K	552.29	Joback Method
cpg	277.93	J/mol×K	589.26	Joback Method
cpg	288.81	J/mol×K	626.23	Joback Method
cpg	299.08	J/mol×K	663.19	Joback Method
cpg	308.77	J/mol×K	700.16	Joback Method
cpg	317.89	J/mol×K	737.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C127750963&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

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
ie:	Ionization energy
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