2,11-Dioxabicyclo[4.4.1]undeca-3,5-dien-10-one, 1,3,7,7-tetramethyl-

Othernames: 1,3,7,7-Tetramethyl-2,11-dioxabicyclo[4.4.1]undeca-3,5-dien-10-one
Inchi: InChI=1S/C13H18O3/c1-9-5-6-11-12(2,3)8-7-10(14)13(4,15-9)16-11/h5-6H,7-8H2,1-4H3
InchiKey: ZYBHCGAHPGDGLE-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: CC1=CC=C2OC(C)(O1)C(=O)CCC2(C)C
Mol. weight [g/mol]: 222.28
CAS: 70412-52-1

Physical Properties

Property code	Value	Unit	Source
gf	-145.57	kJ/mol	Joback Method
hf	-475.45	kJ/mol	Joback Method
hfus	19.73	kJ/mol	Joback Method
hvap	58.09	kJ/mol	Joback Method
ie	7.40	eV	NIST Webbook
ie	7.93	eV	NIST Webbook
log10ws	-3.57		Crippen Method
logp	2.926		Crippen Method
mcvol	177.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
tb	662.15	K	Joback Method
tc	914.62	K	Joback Method
tf	450.27	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.94	J/mol×K	662.15	Joback Method
cpg	515.90	J/mol×K	704.23	Joback Method
cpg	534.07	J/mol×K	746.31	Joback Method
cpg	551.72	J/mol×K	788.38	Joback Method
cpg	569.14	J/mol×K	830.46	Joback Method
cpg	586.59	J/mol×K	872.54	Joback Method

cpg	604.36	J/mol×K	914.62	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=C70412521&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
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