Dispiro[5.1.5.1]tetradecane-7,14-dione

Other names: Cyclohexylketene dimer
Inchi: InChI=1S/C14H20O2/c15-11-13(7-3-1-4-8-13)12(16)14(11)9-5-2-6-10-14/h1-10H2
InchiKey: NQCABGRZRRCWPC-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: O=C1C2(CCCCC2)C(=O)C12CCCCC2
Mol. weight [g/mol]: 220.31
CAS: 950-21-0

Physical Properties

Property code	Value	Unit	Source
gf	-59.70	kJ/mol	Joback Method
hf	-369.27	kJ/mol	Joback Method
hfus	1.27	kJ/mol	Joback Method
hvap	53.86	kJ/mol	Joback Method
ie	9.00 ± 0.05	eV	NIST Webbook
log10ws	-3.44		Crippen Method
logp	3.039		Crippen Method
mcvol	178.680	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
tb	702.08	K	Joback Method
tc	980.38	K	Joback Method
tf	472.24	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.68	J/mol×K	702.08	Joback Method
cpg	573.37	J/mol×K	748.46	Joback Method
cpg	596.11	J/mol×K	794.85	Joback Method
cpg	618.31	J/mol×K	841.23	Joback Method
cpg	640.39	J/mol×K	887.62	Joback Method
cpg	662.77	J/mol×K	934.00	Joback Method
cpg	685.88	J/mol×K	980.38	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=C950210&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
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