Oxacyclotetradecane-2,11-dione, 13-methyl-

Other names: 13-Methyloxacyclotetradecane-2,11-dione
Inchi: InChI=1S/C14H24O3/c1-12-10-13(15)8-6-4-2-3-5-7-9-14(16)17-11-12/h12H,2-11H2,1H3
InchiKey: UXFNPDNBDMXQNY-UHFFFAOYSA-N
Formula: C14H24O3
SMILES: CC1COC(=O)CCCCCCCCC(=O)C1
Mol. weight [g/mol]: 240.34
CAS: 74685-36-2

Physical Properties

Property code	Value	Unit	Source
gf	-336.65	kJ/mol	Joback Method
hf	-734.65	kJ/mol	Joback Method
hfus	14.05	kJ/mol	Joback Method
hvap	61.57	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.259		Crippen Method
mcvol	206.270	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	2137.00		NIST Webbook
rinpol	2137.00		NIST Webbook
rinpol	2140.00		NIST Webbook
tb	736.02	K	Joback Method
tc	1004.20	K	Joback Method
tf	389.77	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.13	J/mol×K	736.02	Joback Method
cpg	671.44	J/mol×K	780.72	Joback Method
cpg	695.09	J/mol×K	825.41	Joback Method
cpg	715.89	J/mol×K	870.11	Joback Method
cpg	733.69	J/mol×K	914.81	Joback Method

cpg	748.31	J/mol×K	959.51	Joback Method
cpg	759.61	J/mol×K	1004.20	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=C74685362&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume