(3E,10Z)-Oxacyclotrideca-3,10-diene-2,7-dione

Inchi: InChI=1S/C12H16O3/c13-11-7-3-1-2-6-10-15-12(14)9-5-4-8-11/h1-2,5,9H,3-4,6-8,10H2/b
InchiKey: QPFMJNUWOHGONF-RLKBUKNLSA-N
Formula: C12H16O3
SMILES: O=C1CCC=CCCOC(=O)C=CCC1
Mol. weight [g/mol]: 208.25
CAS: 144403-15-6

Physical Properties

Property code	Value	Unit	Source
gf	-273.76	kJ/mol	Joback Method
hf	-551.31	kJ/mol	Joback Method
hfus	12.34	kJ/mol	Joback Method
hvap	57.84	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.175		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1737.80		NIST Webbook
tb	688.98	K	Joback Method
tc	967.11	K	Joback Method
tf	376.51	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.44	J/mol×K	688.98	Joback Method
cpg	500.24	J/mol×K	735.33	Joback Method
cpg	520.90	J/mol×K	781.69	Joback Method
cpg	539.24	J/mol×K	828.04	Joback Method
cpg	555.12	J/mol×K	874.40	Joback Method
cpg	568.37	J/mol×K	920.75	Joback Method
cpg	578.83	J/mol×K	967.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C144403156&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
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