2H-Cycloprop[c]indene-2,3(3ah)-dione, hexahydro-3a,7,7-trimethyl-

Other names: 1H-Cycloprop[c]indene-2,3(1aH,3aH)-dione, tetrahydro-3a,7,7-trimethyl-
Inchi: InChI=1S/C13H18O2/c1-11(2)5-4-6-12(3)10(15)9(14)8-7-13(8,11)12/h8H,4-7H2,1-3H3
InchiKey: PHZJSNXIYHJVLI-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CC1(C)CCCC2(C)C(=O)C(=O)C3CC312
Mol. weight [g/mol]: 206.28
CAS: 96678-99-8

Physical Properties

Property code	Value	Unit	Source
gf	-40.63	kJ/mol	Joback Method
hf	-349.43	kJ/mol	Joback Method
hfus	2.93	kJ/mol	Joback Method
hvap	49.17	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.361		Crippen Method
mcvol	164.590	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	1562.80		NIST Webbook
rinpol	1562.80		NIST Webbook
tb	653.02	K	Joback Method
tc	912.93	K	Joback Method
tf	490.47	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.92	J/mol×K	653.02	Joback Method
cpg	506.72	J/mol×K	696.34	Joback Method
cpg	525.93	J/mol×K	739.66	Joback Method
cpg	545.07	J/mol×K	782.98	Joback Method
cpg	564.65	J/mol×K	826.29	Joback Method
cpg	585.18	J/mol×K	869.61	Joback Method

cpg	607.18	J/mol×K	912.93	Joback Method

Sources

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=C96678998&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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