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]: 206.29

Physical Properties

Property code	Value	Unit	Source
hfus	2.93	kJ/mol	Joback Method
logp	2.361		Crippen Method
mcvol	164.590	ml/mol	McGowan Method
rinpol	1562.80		NIST Webbook
rinpol	1562.80		NIST Webbook

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96678998&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices