Cantharidin

Other names: 4,7-Epoxyisobenzofuran-1,3-dione, hexahydro-3a,7a-dimethyl-, (3a«alpha», 4«beta», 7«beta», 7a«alpha»)-
7-Oxabicyclo[2.2.1]heptane-2,3-dicarboxylic anhydride, 2,3-dimethyl-
Cantharides camphor
Cantharidine
Cantharone
Kantaridin
1,2-Dimethyl-3,6-epoxyperhydrophthalic anhydride
exo-1,2-cis-Dimethyl-3,6-epoxyhexahydrophthalic anhydride
CAN
Hexahydro-3a,7a-dimethyl-4,7-epoxyisobenzofuran-1,3-dione
2,3-Dimethyl-7-oxabicyclo(2.2.1)heptane-2,3-dicarboxylic anhydride
4,7-Epoxyisobenzofuran-1,3-dione, hexahydro-3a,7a-dimethyl-
Kantharidin
4,7-Epoxyisobenzofuran-1,3-dione, hexahydro-3a,7a-dimethyl-, (3aR,4S,7R,7aS)-rel-
NSC 61805
CAN [Alkaloid]
(1R,2S,3R,6S)-1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboxylic anhydride

Inchi: InChI=1S/C10H12O4/c1-9-5-3-4-6(13-5)10(9,2)8(12)14-7(9)11/h5-6H,3-4H2,1-2H3/t5-,6-
InchiKey: DHZBEENLJMYSHQ-XCVPVQRUSA-N
Formula: C10H12O4
SMILES: CC12C(=O)OC(=O)C1(C)C1CCC2O1
Mol. weight [g/mol]: 196.20
CAS: 56-25-7

Physical Properties

Property code	Value	Unit	Source
gf	-232.64	kJ/mol	Joback Method
hf	-566.75	kJ/mol	Joback Method
hfus	17.41	kJ/mol	Joback Method
hvap	52.67	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	0.644		Crippen Method
mcvol	134.060	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	1472.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1457.00		NIST Webbook

rinpol	1468.00		NIST Webbook
tb	638.04	K	Joback Method
tc	897.24	K	Joback Method
tf	485.90	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.66	J/mol×K	638.04	Joback Method
cpg	414.97	J/mol×K	681.24	Joback Method
cpg	430.55	J/mol×K	724.44	Joback Method
cpg	445.73	J/mol×K	767.64	Joback Method
cpg	460.86	J/mol×K	810.84	Joback Method
cpg	476.26	J/mol×K	854.04	Joback Method
cpg	492.27	J/mol×K	897.24	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=C56257&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
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