

Chrysanthenone epoxide

Inchi:	InChI=1S/C10H14O2/c1-9(2)5-4-6-10(3,12-6)8(9)7(5)11/h5-6,8H,4H2,1-3H3
InchiKey:	MJKUEDLCFFNGOC-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	CC1(C)C2CC3OC3(C)C1C2=O
Mol. weight [g/mol]:	166.22

Physical Properties

Property code	Value	Unit	Source
gf	-7.44	kJ/mol	Joback Method
hf	-305.07	kJ/mol	Joback Method
hfus	15.20	kJ/mol	Joback Method
hvap	43.26	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.389		Crippen Method
mcvol	126.620	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
rinpol	1317.00		NIST Webbook
tb	530.06	K	Joback Method
tc	761.15	K	Joback Method
tf	393.91	K	Joback Method
vc	0.496	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.67	J/mol×K	530.06	Joback Method
cpg	358.43	J/mol×K	568.57	Joback Method
cpg	373.80	J/mol×K	607.09	Joback Method
cpg	388.07	J/mol×K	645.60	Joback Method
cpg	401.55	J/mol×K	684.12	Joback Method
cpg	414.51	J/mol×K	722.63	Joback Method
cpg	427.26	J/mol×K	761.15	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=R427788&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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