Chrysanthenyl angelate

Inchi: InChI=1S/C15H22O2/c1-6-9(2)14(16)17-13-11-8-7-10(3)12(13)15(11,4)5/h6-7,11-13H,8H
InchiKey: XBIYGXBPWHLVBE-TWGQIWQCSA-N
Formula: C15H22O2
SMILES: CC=C(C)C(=O)OC1C2CC=C(C)C1C2(C)C
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	21.99	kJ/mol	Joback Method
hf	-329.99	kJ/mol	Joback Method
hfus	27.13	kJ/mol	Joback Method
hvap	57.36	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.487		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1535.00		NIST Webbook
tb	635.72	K	Joback Method
tc	848.11	K	Joback Method
tf	372.99	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.17	J/mol×K	635.72	Joback Method
cpg	571.86	J/mol×K	671.12	Joback Method
cpg	589.55	J/mol×K	706.52	Joback Method
cpg	606.41	J/mol×K	741.92	Joback Method
cpg	622.57	J/mol×K	777.32	Joback Method
cpg	638.18	J/mol×K	812.71	Joback Method
cpg	653.38	J/mol×K	848.11	Joback Method

Sources

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=R342320&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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