cis-Chrysanthenyl propionate

Inchi: InChI=1S/C13H20O2/c1-5-10(14)15-12-9-7-6-8(2)11(12)13(9,3)4/h6,9,11-12H,5,7H2,1-4
InchiKey: IRFLZVJYCZYXNP-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CCC(=O)OC1C2CC=C(C)C1C2(C)C
Mol. weight [g/mol]: 208.30
CAS: 70470-69-8

Physical Properties

Property code	Value	Unit	Source
gf	-66.52	kJ/mol	Joback Method
hf	-396.14	kJ/mol	Joback Method
hfus	23.06	kJ/mol	Joback Method
hvap	52.87	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.930		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1354.00		NIST Webbook
rinpol	1354.70		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1354.70		NIST Webbook
rinpol	1343.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1664.00		NIST Webbook
tb	585.92	K	Joback Method
tc	792.95	K	Joback Method
tf	369.49	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.87	J/mol×K	585.92	Joback Method
cpg	487.80	J/mol×K	620.43	Joback Method

cpg	504.74	J/mol×K	654.93	Joback Method
cpg	520.81	J/mol×K	689.44	Joback Method
cpg	536.12	J/mol×K	723.94	Joback Method
cpg	550.78	J/mol×K	758.45	Joback Method
cpg	564.91	J/mol×K	792.95	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=C70470698&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume