cis-Chrysanthenyl pentanoate

Inchi: InChI=1S/C15H24O2/c1-5-6-7-12(16)17-14-11-9-8-10(2)13(14)15(11,3)4/h8,11,13-14H,5
InchiKey: VTUXPTJOYLXSHN-MKDGSZCOSA-N
Formula: C15H24O2
SMILES: CCCCC(=O)OC1C2CC=C(C)C1C2(C)C
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-49.68	kJ/mol	Joback Method
hf	-437.42	kJ/mol	Joback Method
hfus	28.24	kJ/mol	Joback Method
hvap	57.32	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.711		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	1500.00		NIST Webbook
tb	631.68	K	Joback Method
tc	832.71	K	Joback Method
tf	392.03	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.22	J/mol×K	631.68	Joback Method
cpg	593.04	J/mol×K	665.19	Joback Method
cpg	610.92	J/mol×K	698.69	Joback Method
cpg	627.99	J/mol×K	732.20	Joback Method
cpg	644.35	J/mol×K	765.70	Joback Method
cpg	660.11	J/mol×K	799.21	Joback Method
cpg	675.39	J/mol×K	832.71	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=R81378&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