cis-Chrysanthenyl butanoate

Inchi: InChI=1S/C14H22O2/c1-5-6-11(15)16-13-10-8-7-9(2)12(13)14(10,3)4/h7,10,12-13H,5-6,
InchiKey: HGTWZXWLAFIIDA-LQNXFFKNSA-N
Formula: C14H22O2
SMILES: CCCC(=O)OC1C2CC=C(C)C1C2(C)C
Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	-58.10	kJ/mol	Joback Method
hf	-416.78	kJ/mol	Joback Method
hfus	25.65	kJ/mol	Joback Method
hvap	55.10	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.320		Crippen Method
mcvol	189.540	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	1440.00		NIST Webbook
rinpol	1440.00		NIST Webbook
tb	608.80	K	Joback Method
tc	812.71	K	Joback Method
tf	380.76	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.33	J/mol×K	608.80	Joback Method
cpg	539.72	J/mol×K	642.78	Joback Method
cpg	557.16	J/mol×K	676.77	Joback Method
cpg	573.75	J/mol×K	710.75	Joback Method
cpg	589.61	J/mol×K	744.74	Joback Method
cpg	604.84	J/mol×K	778.72	Joback Method
cpg	619.56	J/mol×K	812.71	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=R81346&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