cis-Chrysanthenyl isobutyrate

Inchi: InChI=1S/C14H22O2/c1-8(2)13(15)16-12-10-7-6-9(3)11(12)14(10,4)5/h6,8,10-12H,7H2,1
InchiKey: OSMPHXXLRXFVBK-WIKAKEFZSA-N
Formula: C14H22O2
SMILES: CC1=CCC2C(OC(=O)C(C)C)C1C2(C)C
Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	-60.54	kJ/mol	Joback Method
hf	-422.06	kJ/mol	Joback Method
hfus	22.13	kJ/mol	Joback Method
hvap	54.71	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.176		Crippen Method
mcvol	189.540	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1400.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1668.00		NIST Webbook
tb	608.36	K	Joback Method
tc	816.32	K	Joback Method
tf	365.76	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.70	J/mol×K	608.36	Joback Method
cpg	540.52	J/mol×K	643.02	Joback Method
cpg	558.32	J/mol×K	677.68	Joback Method
cpg	575.24	J/mol×K	712.34	Joback Method
cpg	591.38	J/mol×K	747.00	Joback Method
cpg	606.88	J/mol×K	781.66	Joback Method
cpg	621.85	J/mol×K	816.32	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=R81350&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
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