cis-Chrysanthenyl formate

Inchi: InChI=1S/C11H16O2/c1-7-4-5-8-10(13-6-12)9(7)11(8,2)3/h4,6,8-10H,5H2,1-3H3
InchiKey: UUPONGFJZWADRE-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: CC1=CCC2C(OC=O)C1C2(C)C
Mol. weight [g/mol]: 180.24
CAS: 241123-18-2

Physical Properties

Property code	Value	Unit	Source
gf	-53.96	kJ/mol	Joback Method
hf	-327.86	kJ/mol	Joback Method
hfus	18.57	kJ/mol	Joback Method
hvap	48.39	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.150		Crippen Method
mcvol	147.270	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	1190.30		NIST Webbook
rinpol	1190.30		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1177.00		NIST Webbook
tb	534.95	K	Joback Method
tc	743.67	K	Joback Method
tf	339.02	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.07	J/mol×K	534.95	Joback Method
cpg	388.51	J/mol×K	569.74	Joback Method
cpg	403.93	J/mol×K	604.52	Joback Method
cpg	418.45	J/mol×K	639.31	Joback Method
cpg	432.18	J/mol×K	674.10	Joback Method

cpg	445.24	J/mol×K	708.88	Joback Method
cpg	457.74	J/mol×K	743.67	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=C241123182&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume