Chrysanthenyl propanoate

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

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
ripol	1599.00		NIST Webbook
ripol	1599.00		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=R236809&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume