Chrysanthenyl hexanoate

Inchi: InChI=1S/C16H26O2/c1-5-6-7-8-13(17)18-15-12-10-9-11(2)14(15)16(12,3)4/h9,12,14-15
InchiKey: BYHBSLCRLQTEFD-UHFFFAOYSA-N
Formula: C16H26O2
SMILES: CCCCCC(=O)OC1C2CC=C(C)C1C2(C)C
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	-41.26	kJ/mol	Joback Method
hf	-458.06	kJ/mol	Joback Method
hfus	30.83	kJ/mol	Joback Method
hvap	59.55	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	4.101		Crippen Method
mcvol	217.720	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	1589.00		NIST Webbook
rinpol	1589.00		NIST Webbook
tb	654.56	K	Joback Method
tc	853.02	K	Joback Method
tf	403.30	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.48	J/mol×K	654.56	Joback Method
cpg	647.68	J/mol×K	687.64	Joback Method
cpg	665.98	J/mol×K	720.71	Joback Method
cpg	683.50	J/mol×K	753.79	Joback Method
cpg	700.33	J/mol×K	786.87	Joback Method
cpg	716.59	J/mol×K	819.94	Joback Method
cpg	732.39	J/mol×K	853.02	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=R516026&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