Chrysanthenyl isovalerate

Inchi: InChI=1S/C15H24O2/c1-9(2)8-12(16)17-14-11-7-6-10(3)13(14)15(11,4)5/h6,9,11,13-14H
InchiKey: VCFDIPBWQNPUTA-UHFFFAOYSA-N
Formula: C15H24O2
SMILES: CC1=CCC2C(OC(=O)CC(C)C)C1C2(C)C
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-52.12	kJ/mol	Joback Method
hf	-442.70	kJ/mol	Joback Method
hfus	24.72	kJ/mol	Joback Method
hvap	56.93	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.567		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1452.00		NIST Webbook
tb	631.24	K	Joback Method
tc	836.07	K	Joback Method
tf	377.03	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.62	J/mol×K	631.24	Joback Method
cpg	593.83	J/mol×K	665.38	Joback Method
cpg	612.08	J/mol×K	699.52	Joback Method
cpg	629.46	J/mol×K	733.66	Joback Method
cpg	646.10	J/mol×K	767.80	Joback Method
cpg	662.12	J/mol×K	801.94	Joback Method
cpg	677.64	J/mol×K	836.07	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=R342335&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