Santolinyl acetate

Inchi: InChI=1S/C12H20O2/c1-7-11(8-9(2)3)12(5,6)14-10(4)13/h7-8,11H,1H2,2-6H3
InchiKey: NHUKUXHBUOLLAY-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: C=CC(C=C(C)C)C(C)(C)OC(C)=O
Mol. weight [g/mol]: 196.29
CAS: 79507-88-3

Physical Properties

Property code	Value	Unit	Source
gf	-23.85	kJ/mol	Joback Method
hf	-316.98	kJ/mol	Joback Method
hfus	16.30	kJ/mol	Joback Method
hvap	49.15	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.096		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1171.00		NIST Webbook
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tb	547.30	K	Joback Method
tc	744.21	K	Joback Method
tf	263.78	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.09	J/mol×K	547.30	Joback Method
cpg	445.42	J/mol×K	580.12	Joback Method
cpg	460.82	J/mol×K	612.94	Joback Method
cpg	475.36	J/mol×K	645.76	Joback Method
cpg	489.07	J/mol×K	678.57	Joback Method
cpg	501.99	J/mol×K	711.39	Joback Method
cpg	514.17	J/mol×K	744.21	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=C79507883&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