eupatoriochromene

Inchi: InChI=1S/C13H14O3/c1-8(14)10-6-9-4-5-13(2,3)16-12(9)7-11(10)15/h4-7,15H,1-3H3
InchiKey: SVUVYHFYZBCYRF-UHFFFAOYSA-N
Formula: C13H14O3
SMILES: CC(=O)c1cc2c(cc1O)OC(C)(C)C=C2
Mol. weight [g/mol]: 218.25

Physical Properties

Property code	Value	Unit	Source
gf	-144.81	kJ/mol	Joback Method
hf	-380.29	kJ/mol	Joback Method
hfus	29.01	kJ/mol	Joback Method
hvap	71.63	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.779		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1759.00		NIST Webbook
rinpol	1759.00		NIST Webbook
tb	705.33	K	Joback Method
tc	951.07	K	Joback Method
tf	515.03	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.88	J/mol×K	705.33	Joback Method
cpg	472.21	J/mol×K	746.29	Joback Method
cpg	485.07	J/mol×K	787.24	Joback Method
cpg	497.71	J/mol×K	828.20	Joback Method
cpg	510.37	J/mol×K	869.15	Joback Method
cpg	523.31	J/mol×K	910.11	Joback Method
cpg	536.78	J/mol×K	951.07	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R429224&Units=SI

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