Encecalin

Other names: Encecalin (methyleupatoriochromene)
Encecaline
Inchi: InChI=1S/C14H16O3/c1-9(15)11-7-10-5-6-14(2,3)17-12(10)8-13(11)16-4/h5-8H,1-4H3
InchiKey: WXVLCNREBFDEKS-UHFFFAOYSA-N
Formula: C14H16O3
SMILES: COc1cc2c(cc1C(C)=O)C=CC(C)(C)O2
Mol. weight [g/mol]: 232.28

Physical Properties

Property code	Value	Unit	Source
gf	-96.40	kJ/mol	Joback Method
hf	-367.31	kJ/mol	Joback Method
hfus	26.62	kJ/mol	Joback Method
hvap	63.91	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.082		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1829.00		NIST Webbook
rinpol	1829.00		NIST Webbook
ripol	2607.00		NIST Webbook
ripol	2607.00		NIST Webbook
tb	674.99	K	Joback Method
tc	905.59	K	Joback Method
tf	449.33	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.67	J/mol×K	674.99	Joback Method
cpg	499.79	J/mol×K	713.42	Joback Method
cpg	514.17	J/mol×K	751.86	Joback Method
cpg	527.94	J/mol×K	790.29	Joback Method

cpg	541.25	J/mol×K	828.73	Joback Method
cpg	554.24	J/mol×K	867.16	Joback Method
cpg	567.03	J/mol×K	905.59	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=R37688&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume