Hispaglabridin A

Inchi: InChI=1S/C25H28O4/c1-15(2)5-7-19-21(26)9-8-18(23(19)27)17-13-16-6-10-22-20(24(16
InchiKey: HZHXMXSXYQCAIG-UHFFFAOYSA-N
Formula: C25H28O4
SMILES: CC(C)=CCc1c(O)ccc(C2COc3c(ccc4c3C=CC(C)(C)O4)C2)c1O
Mol. weight [g/mol]: 392.49
CAS: 68978-03-0

Physical Properties

Property code	Value	Unit	Source
gf	57.88	kJ/mol	Joback Method
hf	-437.04	kJ/mol	Joback Method
hfus	60.44	kJ/mol	Joback Method
hvap	112.84	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.509		Crippen Method
mcvol	308.750	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	3455.90		NIST Webbook
rinpol	3455.90		NIST Webbook
tb	1085.28	K	Joback Method
tc	1350.55	K	Joback Method
tf	785.47	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.82	J/mol×K	1085.28	Joback Method
cpg	1140.04	J/mol×K	1129.49	Joback Method
cpg	1175.16	J/mol×K	1173.70	Joback Method
cpg	1213.67	J/mol×K	1217.92	Joback Method
cpg	1256.10	J/mol×K	1262.13	Joback Method
cpg	1302.94	J/mol×K	1306.34	Joback Method
cpg	1354.70	J/mol×K	1350.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68978030&Units=SI
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

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