

Hispaglabridin B

Inchi:	InChI=1S/C25H26O4/c1-24(2)11-9-18-20(28-24)8-6-17(22(18)26)16-13-15-5-7-21-19(23
InchiKey:	CJUFYKORDZSOLF-UHFFFAOYSA-N
Formula:	C25H26O4
SMILES:	CC1(C)C=Cc2c(ccc(C3COc4c(ccc5c4C=CC(C)(C)O5)C3)c2O)O1
Mol. weight [g/mol]:	390.47
CAS:	68978-02-9

Physical Properties

Property code	Value	Unit	Source
gf	118.20	kJ/mol	Joback Method
hf	-370.97	kJ/mol	Joback Method
hfus	54.32	kJ/mol	Joback Method
hvap	104.19	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	5.479		Crippen Method
mcvol	297.890	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	3273.30		NIST Webbook
rinpol	3273.30		NIST Webbook
tb	1042.96	K	Joback Method
tc	1314.09	K	Joback Method
tf	770.96	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.93	J/molxK	1042.96	Joback Method
cpg	1099.81	J/molxK	1088.15	Joback Method
cpg	1138.20	J/molxK	1133.34	Joback Method
cpg	1180.72	J/molxK	1178.53	Joback Method
cpg	1227.99	J/molxK	1223.72	Joback Method
cpg	1280.64	J/molxK	1268.91	Joback Method
cpg	1339.31	J/molxK	1314.09	Joback Method

Sources

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=C68978029&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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