3'-Hydroxy-4'-O-methylglabridin

Inchi: InChI=1S/C21H22O5/c1-21(2)9-8-15-16(26-21)6-4-12-10-13(11-25-20(12)15)14-5-7-17(2
InchiKey: PPBISUGOQDBBEL-UHFFFAOYSA-N
Formula: C21H22O5
SMILES: COc1ccc(C2COc3c(ccc4c3C=CC(C)(C)O4)C2)c(O)c1O
Mol. weight [g/mol]: 354.40
CAS: 175554-11-7

Physical Properties

Property code	Value	Unit	Source
gf	-152.47	kJ/mol	Joback Method
hf	-594.13	kJ/mol	Joback Method
hfus	52.38	kJ/mol	Joback Method
hvap	106.31	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.009		Crippen Method
mcvol	262.560	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	3123.20		NIST Webbook
rinpol	3123.20		NIST Webbook
tb	1012.14	K	Joback Method
tc	1277.10	K	Joback Method
tf	781.66	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.43	J/mol×K	1012.14	Joback Method
cpg	925.88	J/mol×K	1056.30	Joback Method
cpg	952.13	J/mol×K	1100.46	Joback Method
cpg	980.59	J/mol×K	1144.62	Joback Method
cpg	1011.71	J/mol×K	1188.78	Joback Method
cpg	1045.90	J/mol×K	1232.94	Joback Method
cpg	1083.59	J/mol×K	1277.10	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=C175554117&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