4'-O-Methylglabridin

Inchi: InChI=1S/C21H22O4/c1-21(2)9-8-17-19(25-21)7-4-13-10-14(12-24-20(13)17)16-6-5-15(2
InchiKey: ZZAIPFIGEGQNHP-UHFFFAOYSA-N
Formula: C21H22O4
SMILES: COc1ccc(C2COc3c(ccc4c3C=CC(C)(C)O4)C2)c(O)c1
Mol. weight [g/mol]: 338.40
CAS: 68978-09-6

Physical Properties

Property code	Value	Unit	Source
gf	2.15	kJ/mol	Joback Method
hf	-416.82	kJ/mol	Joback Method
hfus	46.60	kJ/mol	Joback Method
hvap	93.30	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.304		Crippen Method
mcvol	256.690	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	3046.70		NIST Webbook
rinpol	3046.70		NIST Webbook
tb	931.52	K	Joback Method
tc	1190.83	K	Joback Method
tf	669.94	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.80	J/mol×K	931.52	Joback Method
cpg	860.34	J/mol×K	974.74	Joback Method
cpg	881.36	J/mol×K	1017.96	Joback Method
cpg	903.18	J/mol×K	1061.17	Joback Method
cpg	926.14	J/mol×K	1104.39	Joback Method
cpg	950.57	J/mol×K	1147.61	Joback Method
cpg	976.81	J/mol×K	1190.83	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=C68978096&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume