1,3-Benzenediol, 4-[(3R)-3,4-dihydro-8,8-dimethyl-2H,8H-benzo[1,2-

Other names: Glabridin
Inchi: InChI=1S/C20H20O4/c1-20(2)8-7-16-18(24-20)6-3-12-9-13(11-23-19(12)16)15-5-4-14(21
InchiKey: LBQIJVLKGVZRIW-UHFFFAOYSA-N
Formula: C20H20O4
SMILES: CC1(C)C=Cc2c(ccc3c2OCC(c2ccc(O)cc2O)C3)O1
Mol. weight [g/mol]: 324.37
CAS: 59870-68-7

Physical Properties

Property code	Value	Unit	Source
gf	-46.26	kJ/mol	Joback Method
hf	-429.80	kJ/mol	Joback Method
hfus	48.99	kJ/mol	Joback Method
hvap	101.01	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.001		Crippen Method
mcvol	242.600	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinpol	3127.50		NIST Webbook
rinpol	3127.50		NIST Webbook
tb	961.86	K	Joback Method
tc	1233.73	K	Joback Method
tf	735.64	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.92	J/mol×K	961.86	Joback Method
cpg	831.61	J/mol×K	1007.17	Joback Method
cpg	856.03	J/mol×K	1052.48	Joback Method
cpg	882.68	J/mol×K	1097.80	Joback Method
cpg	912.04	J/mol×K	1143.11	Joback Method
cpg	944.63	J/mol×K	1188.42	Joback Method

cpg	980.93	J/mol×K	1233.73	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=C59870687&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