

Glabrol

Inchi:	InChI=1S/C25H28O4/c1-15(2)5-7-17-13-18(8-11-21(17)26)24-14-23(28)20-10-12-22(27)
InchiKey:	CUFAXDWQDQKFF-UHFFFAOYSA-N
Formula:	C25H28O4
SMILES:	<chem>CC(C)=CCc1cc(C2CC(=O)c3ccc(O)c(CC=C(C)C)c3O2)ccc1O</chem>
Mol. weight [g/mol]:	392.49
CAS:	59870-65-4

Physical Properties

Property code	Value	Unit	Source
gf	29.59	kJ/mol	Joback Method
hf	-463.50	kJ/mol	Joback Method
hfus	60.30	kJ/mol	Joback Method
hvap	112.73	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	5.822		Crippen Method
mcvol	315.310	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	3424.30		NIST Webbook
rinpol	3424.30		NIST Webbook
tb	1114.80	K	Joback Method
tc	1378.38	K	Joback Method
tf	756.48	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1102.35	J/molxK	1114.80	Joback Method
cpg	1124.40	J/molxK	1158.73	Joback Method
cpg	1147.23	J/molxK	1202.66	Joback Method
cpg	1171.13	J/molxK	1246.59	Joback Method
cpg	1196.38	J/molxK	1290.52	Joback Method
cpg	1223.28	J/molxK	1334.45	Joback Method
cpg	1252.12	J/molxK	1378.38	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C59870654&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
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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