(.+/-.)-Demethylsalvicanol

Inchi: InChI=1S/C20H30O3/c1-12(2)14-10-13-6-7-16-19(3,4)8-5-9-20(16,23)11-15(13)18(22)17
InchiKey: XZANDTPHDIYTME-UHFFFAOYSA-N
Formula: C20H30O3
SMILES: CC(C)c1cc2c(c(O)c1O)CC1(O)CCCC(C)(C)C1CC2
Mol. weight [g/mol]: 318.45
CAS: 177019-45-3

Physical Properties

Property code	Value	Unit	Source
gf	-171.32	kJ/mol	Joback Method
hf	-617.41	kJ/mol	Joback Method
hfus	31.39	kJ/mol	Joback Method
hvap	103.76	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.267		Crippen Method
mcvol	264.790	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	2641.10		NIST Webbook
rinpol	2641.10		NIST Webbook
tb	968.72	K	Joback Method
tc	1209.99	K	Joback Method
tf	704.76	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.04	J/mol×K	968.72	Joback Method
cpg	983.13	J/mol×K	1008.93	Joback Method
cpg	1013.42	J/mol×K	1049.14	Joback Method
cpg	1046.34	J/mol×K	1089.36	Joback Method
cpg	1082.35	J/mol×K	1129.57	Joback Method
cpg	1121.89	J/mol×K	1169.78	Joback Method
cpg	1165.43	J/mol×K	1209.99	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=C177019453&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