Pisiferol

Inchi: InChI=1S/C20H30O2/c1-13(2)15-10-14-6-7-18-19(3,4)8-5-9-20(18,12-21)16(14)11-17(15
InchiKey: NKGGFTFDYGTUSL-UHFFFAOYSA-N
Formula: C20H30O2
SMILES: CC(C)c1cc2c(cc1O)C1(CO)CCCC(C)(C)C1CC2
Mol. weight [g/mol]: 302.45
CAS: 24035-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-4.60	kJ/mol	Joback Method
hf	-433.94	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	90.58	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.518		Crippen Method
mcvol	258.920	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	2615.40		NIST Webbook
rinpol	2615.40		NIST Webbook
tb	883.83	K	Joback Method
tc	1112.08	K	Joback Method
tf	596.56	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.53	J/mol×K	883.83	Joback Method
cpg	902.42	J/mol×K	921.87	Joback Method
cpg	926.17	J/mol×K	959.91	Joback Method
cpg	951.14	J/mol×K	997.95	Joback Method
cpg	977.67	J/mol×K	1036.00	Joback Method
cpg	1006.10	J/mol×K	1074.04	Joback Method
cpg	1036.79	J/mol×K	1112.08	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=C24035367&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