Resorcinol, 2-p-mentha-1,8-dien-3-yl-5-pentyl-, (-)-(E)-

Other names: 1,3-Benzenediol, 2-(3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl)-5-pentyl-, (1R-trans)-
Cannabidiol
(-)-trans-Cannabidiol
CBD
(-)-trans-2-p-Mentha-1,8-dien-3-yl-5-pentylresorcinol
2-(6-Isopropenyl-3-methyl-2-cyclohexen-1-yl)-5-pentyl-1,3-benzenediol

Inchi: InChI=1S/C21H30O2/c1-5-6-7-8-16-12-19(22)21(20(23)13-16)18-11-15(4)9-10-17(18)14

InchiKey: QHMBSVQNZZTUGM-MSOLQXFVSA-N

Formula: C21H30O2

SMILES: C=C(C)C1CCC(C)=CC1c1c(O)cc(CCCCC)cc1O

Mol. weight [g/mol]: 314.46

CAS: 521-37-9

Physical Properties

Property code	Value	Unit	Source
gf	35.84	kJ/mol	Joback Method
hf	-410.40	kJ/mol	Joback Method
hfus	46.51	kJ/mol	Joback Method
hvap	91.79	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.846		Crippen Method
mcvol	275.270	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
rinpol	2383.00		NIST Webbook
rinpol	2385.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2383.00		NIST Webbook
rinpol	2441.30		NIST Webbook
rinpol	2392.00		NIST Webbook
rinpol	2366.00		NIST Webbook
tb	888.36	K	Joback Method
tc	1119.73	K	Joback Method
tf	589.51	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.02	J/mol×K	888.36	Joback Method
cpg	920.75	J/mol×K	926.92	Joback Method
cpg	938.84	J/mol×K	965.48	Joback Method
cpg	956.45	J/mol×K	1004.05	Joback Method
cpg	973.76	J/mol×K	1042.61	Joback Method
cpg	990.91	J/mol×K	1081.17	Joback Method
cpg	1008.09	J/mol×K	1119.73	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C521379&Units=SI
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

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