1,3-Benzenediol, 2-(3,7-dimethyl-2,6-octadienyl)-5-pentyl-

Other names: Resorcinol, 2-(3,7-dimethyl-2,6-octadienyl)-5-pentyl-
Cannabigerol

Inchi: InChI=1S/C21H32O2/c1-5-6-7-11-18-14-20(22)19(21(23)15-18)13-12-17(4)10-8-9-16(2)3

InchiKey: QXACEHWTBCFNSA-SFQUDFHCSA-N

Formula: C21H32O2

SMILES: CCCCCc1cc(O)c(CC=C(C)CCC=C(C)C)c(O)c1

Mol. weight [g/mol]: 316.48

CAS: 2808-33-5

Physical Properties

Property code	Value	Unit	Source
gf	62.82	kJ/mol	Joback Method
hf	-391.47	kJ/mol	Joback Method
hfus	53.15	kJ/mol	Joback Method
hvap	91.38	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.066		Crippen Method
mcvol	286.130	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	2496.00		NIST Webbook
tb	880.86	K	Joback Method
tc	1098.77	K	Joback Method
tf	550.73	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.03	J/mol×K	880.86	Joback Method
cpg	924.03	J/mol×K	917.18	Joback Method
cpg	941.75	J/mol×K	953.50	Joback Method
cpg	959.36	J/mol×K	989.82	Joback Method
cpg	977.04	J/mol×K	1026.13	Joback Method
cpg	994.97	J/mol×K	1062.45	Joback Method

cpg	1013.30	J/mol×K	1098.77	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=C2808335&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