

2-Methyl-3,5-diisopropylphenol

Inchi:	InChI=1S/C13H20O/c1-8(2)11-6-12(9(3)4)10(5)13(14)7-11/h6-9,14H,1-5H3
InchiKey:	LNJNFIIJYVIYBA-UHFFFAOYSA-N
Formula:	C13H20O
SMILES:	<chem>Cc1c(O)cc(C(C)C)cc1C(C)C</chem>
Mol. weight [g/mol]:	192.30
CAS:	22292-76-8

Physical Properties

Property code	Value	Unit	Source
chs	-7607.00	kJ/mol	NIST Webbook
gf	-7.77	kJ/mol	Joback Method
hf	-259.00	kJ/mol	NIST Webbook
hfs	-370.00	kJ/mol	NIST Webbook
hfus	21.43	kJ/mol	Joback Method
hsub	109.20	kJ/mol	NIST Webbook
hsub	111.00	kJ/mol	NIST Webbook
hvap	60.37	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.947		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
tb	613.22	K	Joback Method
tc	831.48	K	Joback Method
tf	369.45	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.72	J/molxK	613.22	Joback Method
cpg	526.69	J/molxK	795.10	Joback Method
cpg	513.88	J/molxK	758.72	Joback Method
cpg	500.35	J/molxK	722.35	Joback Method
cpg	486.03	J/molxK	685.97	Joback Method

cpg	470.84	J/mol×K	649.60	Joback Method
cpg	538.86	J/mol×K	831.48	Joback Method
dvisc	0.0000243	Paxs	613.22	Joback Method
dvisc	0.0000389	Paxs	572.59	Joback Method
dvisc	0.0000668	Paxs	531.96	Joback Method
dvisc	0.0001255	Paxs	491.34	Joback Method
dvisc	0.0002640	Paxs	450.71	Joback Method
dvisc	0.0006436	Paxs	410.08	Joback Method
dvisc	0.0019088	Paxs	369.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22292768&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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