

3,5-Diisopropylphenol

Inchi:	InChI=1S/C12H18O/c1-8(2)10-5-11(9(3)4)7-12(13)6-10/h5-9,13H,1-4H3
InchiKey:	YYOQJBLGFMMLRJ-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	CC(C)c1cc(O)cc(C(C)C)c1
Mol. weight [g/mol]:	178.27
CAS:	3374-41-2

Physical Properties

Property code	Value	Unit	Source
chs	-6958.00	kJ/mol	NIST Webbook
gf	-6.56	kJ/mol	Joback Method
hf	-236.00	kJ/mol	NIST Webbook
hfs	-330.00	kJ/mol	NIST Webbook
hfus	19.22	kJ/mol	Joback Method
hsub	94.00	kJ/mol	NIST Webbook
hsub	98.24	kJ/mol	NIST Webbook
hvap	57.48	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.639		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
tb	585.36	K	Joback Method
tc	806.59	K	Joback Method
tf	345.66	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.79	J/mol×K	585.36	Joback Method
cpg	421.56	J/mol×K	622.23	Joback Method
cpg	436.33	J/mol×K	659.10	Joback Method
cpg	450.20	J/mol×K	695.97	Joback Method
cpg	463.24	J/mol×K	732.85	Joback Method

cpg	475.53	J/mol×K	769.72	Joback Method
cpg	487.16	J/mol×K	806.59	Joback Method
dvisc	0.0036943	Pa×s	345.66	Joback Method
dvisc	0.0011103	Pa×s	385.61	Joback Method
dvisc	0.0004182	Pa×s	425.56	Joback Method
dvisc	0.0001862	Pa×s	465.51	Joback Method
dvisc	0.0000943	Pa×s	505.46	Joback Method
dvisc	0.0000527	Pa×s	545.41	Joback Method
dvisc	0.0000319	Pa×s	585.36	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=C3374412&Units=SI

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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