4-Methyl-3,5-diisopropylphenol

Inchi: InChI=1S/C13H20O/c1-8(2)12-6-11(14)7-13(9(3)4)10(12)5/h6-9,14H,1-5H3
InchiKey: XIGWUCHSXAEESN-UHFFFAOYSA-N
Formula: C13H20O
SMILES: Cc1c(C(C)C)cc(O)cc1C(C)C
Mol. weight [g/mol]: 192.30
CAS: 15269-17-7

Physical Properties

Property code	Value	Unit	Source
chs	-7607.00	kJ/mol	NIST Webbook
gf	-7.77	kJ/mol	Joback Method
hf	-257.00	kJ/mol	NIST Webbook
hfs	-370.00	kJ/mol	NIST Webbook
hfus	21.43	kJ/mol	Joback Method
hsub	110.80	kJ/mol	NIST Webbook
hsub	113.00	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/mol×K	613.22	Joback Method
cpg	526.69	J/mol×K	795.10	Joback Method
cpg	513.88	J/mol×K	758.72	Joback Method
cpg	500.35	J/mol×K	722.35	Joback Method
cpg	486.03	J/mol×K	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	Pa×s	613.22	Joback Method
dvisc	0.0000389	Pa×s	572.59	Joback Method
dvisc	0.0000668	Pa×s	531.96	Joback Method
dvisc	0.0001255	Pa×s	491.34	Joback Method
dvisc	0.0002640	Pa×s	450.71	Joback Method
dvisc	0.0006436	Pa×s	410.08	Joback Method
dvisc	0.0019088	Pa×s	369.45	Joback Method

Sources

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=C15269177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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