

3,5-Bis(2-butyl)phenol

Inchi:	InChI=1S/C14H22O/c1-5-10(3)12-7-13(11(4)6-2)9-14(15)8-12/h7-11,15H,5-6H2,1-4H3
InchiKey:	PFBHMJJMZWUEAI-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	CCC(C)c1cc(O)cc(C(C)CC)c1
Mol. weight [g/mol]:	206.32
CAS:	14556-13-9

Physical Properties

Property code	Value	Unit	Source
gf	10.28	kJ/mol	Joback Method
hf	-295.10	kJ/mol	Joback Method
hfus	24.40	kJ/mol	Joback Method
hvap	61.93	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.419		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
tb	631.12	K	Joback Method
tc	844.75	K	Joback Method
tf	368.20	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.95	J/mol×K	631.12	Joback Method
cpg	581.24	J/mol×K	809.14	Joback Method
cpg	567.84	J/mol×K	773.54	Joback Method
cpg	553.68	J/mol×K	737.93	Joback Method
cpg	538.70	J/mol×K	702.33	Joback Method
cpg	522.82	J/mol×K	666.72	Joback Method
cpg	593.96	J/mol×K	844.75	Joback Method
dvisc	0.0000203	Pa×s	631.12	Joback Method
dvisc	0.0000334	Pa×s	587.30	Joback Method

dvisc	0.0000595	Pa×s	543.48	Joback Method
dvisc	0.0001171	Pa×s	499.66	Joback Method
dvisc	0.0002627	Pa×s	455.84	Joback Method
dvisc	0.0006999	Pa×s	412.02	Joback Method
dvisc	0.0023539	Pa×s	368.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14556139&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
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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