

2,4-Bis(1-methylbutyl)phenol

Inchi:	InChI=1S/C16H26O/c1-5-7-12(3)14-9-10-16(17)15(11-14)13(4)8-6-2/h9-13,17H,5-8H2,1
InchiKey:	QEVQVYGCTVKSER-UHFFFAOYSA-N
Formula:	C16H26O
SMILES:	CCCC(C)c1ccc(O)c(C(C)CCC)c1
Mol. weight [g/mol]:	234.38
CAS:	96-94-6

Physical Properties

Property code	Value	Unit	Source
gf	27.12	kJ/mol	Joback Method
hf	-336.38	kJ/mol	Joback Method
hfus	29.59	kJ/mol	Joback Method
hvap	66.39	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	5.199		Crippen Method
mvol	218.410	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
tb	676.88	K	Joback Method
tc	884.07	K	Joback Method
tf	390.74	K	Joback Method
vc	0.777	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.77	J/molxK	676.88	Joback Method
cpg	629.46	J/molxK	711.41	Joback Method
cpg	646.19	J/molxK	745.94	Joback Method
cpg	662.02	J/molxK	780.48	Joback Method
cpg	677.03	J/molxK	815.01	Joback Method
cpg	691.29	J/molxK	849.54	Joback Method
cpg	704.90	J/molxK	884.07	Joback Method
dvisc	0.0015062	Paxs	390.74	Joback Method
dvisc	0.0004441	Paxs	438.43	Joback Method

dvisc	0.0001664	Paxs	486.12	Joback Method
dvisc	0.0000743	Paxs	533.81	Joback Method
dvisc	0.0000379	Paxs	581.50	Joback Method
dvisc	0.0000214	Paxs	629.19	Joback Method
dvisc	0.0000131	Paxs	676.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96946&Units=SI

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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