

Phenol, 2,4-bis(1-phenylethyl)-

Other names:	2,4-bis(1-phenylethyl)phenol
Inchi:	InChI=1S/C22H22O/c1-16(18-9-5-3-6-10-18)20-13-14-22(23)21(15-20)17(2)19-11-7-4-8
InchiKey:	RCFAHSGZAAFQJH-UHFFFAOYSA-N
Formula:	C22H22O
SMILES:	CC(c1ccccc1)c1ccc(O)c(C(C)c2ccccc2)c1
Mol. weight [g/mol]:	302.41
CAS:	2769-94-0

Physical Properties

Property code	Value	Unit	Source
gf	302.46	kJ/mol	Joback Method
hf	12.84	kJ/mol	Joback Method
hfus	33.21	kJ/mol	Joback Method
hvap	84.29	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.696		Crippen Method
mcvol	255.430	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	2426.00		NIST Webbook
tb	867.52	K	Joback Method
tc	1128.60	K	Joback Method
tf	511.20	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.05	J/molxK	867.52	Joback Method
cpg	787.19	J/molxK	911.03	Joback Method
cpg	803.28	J/molxK	954.55	Joback Method
cpg	818.55	J/molxK	998.06	Joback Method
cpg	833.20	J/molxK	1041.57	Joback Method
cpg	847.45	J/molxK	1085.09	Joback Method
cpg	861.52	J/molxK	1128.60	Joback Method

dvisc	0.0001813	Paxs	511.20	Joback Method
dvisc	0.0000652	Paxs	570.59	Joback Method
dvisc	0.0000285	Paxs	629.97	Joback Method
dvisc	0.0000143	Paxs	689.36	Joback Method
dvisc	0.0000080	Paxs	748.75	Joback Method
dvisc	0.0000049	Paxs	808.13	Joback Method
dvisc	0.0000032	Paxs	867.52	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=C2769940&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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