

Phenol, 3-(2-phenylethyl)-

Other names:	Phenol, m-phenethyl- 1-m-Hydroxyphenyl-2-phenylethane 3-(2-Phenylethyl)phenol 1-(3-Hydroxyphenyl)-2-phenylethane
Inchi:	InChI=1S/C14H14O/c15-14-8-4-7-13(11-14)10-9-12-5-2-1-3-6-12/h1-8,11,15H,9-10H2
InchiKey:	AIHZDRMFOVBNAV-UHFFFAOYSA-N
Formula:	C14H14O
SMILES:	Oc1cccc(CCc2ccccc2)c1
Mol. weight [g/mol]:	198.26
CAS:	33675-75-1

Physical Properties

Property code	Value	Unit	Source
gf	137.20	kJ/mol	Joback Method
hf	-36.54	kJ/mol	Joback Method
hfus	25.88	kJ/mol	Joback Method
hvap	64.32	kJ/mol	Joback Method
ie	8.30 ± 0.10	eV	NIST Webbook
log10ws	-3.44		Crippen Method
logp	3.177		Crippen Method
mcvol	166.470	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
rinpol	307.33		NIST Webbook
rinpol	307.33		NIST Webbook
tb	653.70	K	Joback Method
tc	902.41	K	Joback Method
tf	412.10	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.59	J/molxK	653.70	Joback Method
cpg	441.88	J/molxK	695.15	Joback Method

cpg	455.97	J/molxK	736.60	Joback Method
cpg	469.01	J/molxK	778.06	Joback Method
cpg	481.14	J/molxK	819.51	Joback Method
cpg	492.51	J/molxK	860.96	Joback Method
cpg	503.27	J/molxK	902.41	Joback Method
dvisc	0.0009169	Paxs	412.10	Joback Method
dvisc	0.0003694	Paxs	452.37	Joback Method
dvisc	0.0001727	Paxs	492.63	Joback Method
dvisc	0.0000906	Paxs	532.90	Joback Method
dvisc	0.0000520	Paxs	573.17	Joback Method
dvisc	0.0000321	Paxs	613.43	Joback Method
dvisc	0.0000210	Paxs	653.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33675751&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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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