

4-(1-Phenylethyl)phenol

Other names:	Phenol, p-(«alpha»-methylbenzyl)- 1-(4-Hydroxyphenyl)-1-phenylethane 1-Phenyl-1-(4-hydroxyphenyl)ethane 4-(«alpha»-Methylbenzyl)phenol 4-(Phenylethylidene)phenol 4-(1-Phenylethyl)phenol 4-(1-Fenylethyl)fenol p-(«alpha»-Methylbenzyl)phenol Styrolfenol NSC 1859 NSC 60586 p-(1-phenylethyl)phenol
Inchi:	InChI=1S/C14H14O/c1-11(12-5-3-2-4-6-12)13-7-9-14(15)10-8-13/h2-11,15H,1H3
InchiKey:	XHASMJXNUHCHBL-UHFFFAOYSA-N
Formula:	C14H14O
SMILES:	CC(c1ccccc1)c1ccc(O)cc1
Mol. weight [g/mol]:	198.27

Physical Properties

Property code	Value	Unit	Source
af	0.5652		Cheméo Relay (1.0)
gf	134.76	kJ/mol	Joback Method
hf	-18.80	kJ/mol	Cheméo Relay (1.0)
hfus	22.36	kJ/mol	Joback Method
hvap	93.22	kJ/mol	Cheméo Relay (1.0)
ie	8.15	eV	Cheméo Relay (1.0)
log10ws	-3.15		Cheméo Relay (1.0)
logp	3.544		Crippen Method
mcvol	166.470	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
tb	586.83	K	Cheméo Relay (1.0)
tc	857.36	K	Cheméo Relay (1.0)
tf	334.22	K	Cheméo Relay (1.0)
vc	0.578	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.21	J/mol×K	907.43	Joback Method
cpg	482.79	J/mol×K	822.71	Joback Method
cpg	427.10	J/mol×K	653.26	Joback Method
cpg	442.76	J/mol×K	695.62	Joback Method
cpg	457.16	J/mol×K	737.98	Joback Method
cpg	470.46	J/mol×K	780.35	Joback Method
cpg	494.33	J/mol×K	865.07	Joback Method
dvisc	0.0012972	Pa×s	397.10	Joback Method
dvisc	0.0004594	Pa×s	439.79	Joback Method
dvisc	0.0001955	Pa×s	482.49	Joback Method
dvisc	0.0000956	Pa×s	525.18	Joback Method
dvisc	0.0000521	Pa×s	567.87	Joback Method
dvisc	0.0000309	Pa×s	610.57	Joback Method
dvisc	0.0000196	Pa×s	653.26	Joback Method
hvapt	90.80	kJ/mol	482.00	NIST Webbook
hvapt	75.40	kJ/mol	485.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1988892&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
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
h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	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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