

Benzenebutanol

Other names:	1-butanol, 4-phenyl- 4-Phenyl butanol-1 4-Phenyl-n-butanol 4-Phenylbutanol 4-phenyl-1-butanol 4-phenylbutan-1-ol Phenylbutyl alcohol
Inchi:	InChI=1S/C10H14O/c11-9-5-4-8-10-6-2-1-3-7-10/h1-3,6-7,11H,4-5,8-9H2
InchiKey:	LDZLXQFDGRCELX-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	OCCCCc1ccccc1
Mol. weight [g/mol]:	150.22
CAS:	3360-41-6

Physical Properties

Property code	Value	Unit	Source
gf	8.91	kJ/mol	Joback Method
hf	-165.43	kJ/mol	Joback Method
hfus	19.79	kJ/mol	Joback Method
hvap	56.81	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.002		Crippen Method
mvol	133.870	ml/mol	McGowan Method
pc	3070.00	kPa	Vapor-Liquid Critical Properties of Phenol and (C8 to C10) Phenylalkanols
tb	547.06	K	Joback Method
tc	739.47	K	Joback Method
tf	289.70	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	311.72	J/molxK	547.06	Joback Method
cpg	324.22	J/molxK	579.13	Joback Method
cpg	336.04	J/molxK	611.20	Joback Method
cpg	347.19	J/molxK	643.27	Joback Method
cpg	357.73	J/molxK	675.33	Joback Method
cpg	367.66	J/molxK	707.40	Joback Method
cpg	377.01	J/molxK	739.47	Joback Method
dvisc	0.0140109	Paxs	289.70	Joback Method
dvisc	0.0036769	Paxs	332.59	Joback Method
dvisc	0.0013099	Paxs	375.49	Joback Method
dvisc	0.0005766	Paxs	418.38	Joback Method
dvisc	0.0002957	Paxs	461.27	Joback Method
dvisc	0.0001699	Paxs	504.17	Joback Method
dvisc	0.0001065	Paxs	547.06	Joback Method

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3360416&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

Vapor-Liquid Critical Properties of Phenol and (C8 to C10) Phenylalkanols: Partitioning of Phenylalkanols between Micelles and Water Studied by Limiting Joback Method Coefficients in Water and Tetradecyltrimethylammonium Bromide Solutions:

<https://www.doi.org/10.1021/je0604380>

<https://www.doi.org/10.1021/je900967j>

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

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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