

4-Phenyl-2-butanol

Other names:	Benzenepropanol, «alpha»-methyl- «alpha»-Methylbenzenepropanol 4-Phenylbutan-2-ol
Inchi:	InChI=1S/C10H14O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-6,9,11H,7-8H2,1H3
InchiKey:	GDWRKZLROIFUML-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CC(O)CCc1ccccc1
Mol. weight [g/mol]:	150.22
CAS:	2344-70-9

Physical Properties

Property code	Value	Unit	Source
gf	6.47	kJ/mol	Joback Method
hf	-170.71	kJ/mol	Joback Method
hfus	16.26	kJ/mol	Joback Method
hvap	56.42	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.000		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
rinpola	1241.00		NIST Webbook
ripola	2029.00		NIST Webbook
tb	546.62	K	Joback Method
tc	743.00	K	Joback Method
tf	274.70	K	Joback Method
vc	0.500	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.06	J/molxK	546.62	Joback Method
cpg	369.24	J/molxK	710.27	Joback Method
cpg	359.13	J/molxK	677.54	Joback Method
cpg	348.39	J/molxK	644.81	Joback Method

cpg	336.98	J/mol×K	612.08	Joback Method
cpg	324.88	J/mol×K	579.35	Joback Method
cpg	378.75	J/mol×K	743.00	Joback Method
dvisc	0.0001002	Paxs	546.62	Joback Method
dvisc	0.0001658	Paxs	501.30	Joback Method
dvisc	0.0003030	Paxs	455.98	Joback Method
dvisc	0.0006329	Paxs	410.66	Joback Method
dvisc	0.0015868	Paxs	365.34	Joback Method
dvisc	0.0051616	Paxs	320.02	Joback Method
dvisc	0.0247773	Paxs	274.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C2344709&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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