

1-Phenyl-1-butanol

Inchi:	InChI=1S/C10H14O/c1-2-6-10(11)9-7-4-3-5-8-9/h3-5,7-8,10-11H,2,6H2,1H3/t10-/m0/s1
InchiKey:	HQRWWHIETAKIMO-JTQLQIEISA-N
Formula:	C10H14O
SMILES:	CCCC(O)c1ccccc1
Mol. weight [g/mol]:	150.22
CAS:	22144-60-1

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	-2.83		Crippen Method
logp	2.520		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
tb	546.62	K	Joback Method
tc	743.00	K	Joback Method
tf	274.70	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.06	J/mol×K	546.62	Joback Method
cpg	369.24	J/mol×K	710.27	Joback Method
cpg	359.13	J/mol×K	677.54	Joback Method
cpg	348.39	J/mol×K	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	Pa×s	546.62	Joback Method
dvisc	0.0001658	Pa×s	501.30	Joback Method

dvisc	0.0003030	Pa×s	455.98	Joback Method
dvisc	0.0006329	Pa×s	410.66	Joback Method
dvisc	0.0015868	Pa×s	365.34	Joback Method
dvisc	0.0051616	Pa×s	320.02	Joback Method
dvisc	0.0247773	Pa×s	274.70	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.20	K	1.90	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22144601&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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