

Cyclohexanol, 1-butyl-

Other names:	1-n-Butylcyclohexanol 1-Butylcyclohexanol 1-Butylcyclohexanol
Inchi:	InChI=1S/C10H20O/c1-2-3-7-10(11)8-5-4-6-9-10/h11H,2-9H2,1H3
InchiKey:	RCHLXMOXBJRGNX-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CCCCC1(O)CCCCC1
Mol. weight [g/mol]:	156.27
CAS:	5445-30-7

Physical Properties

Property code	Value	Unit	Source
gf	-84.54	kJ/mol	Joback Method
hf	-332.40	kJ/mol	Joback Method
hfus	11.28	kJ/mol	Joback Method
hvap	53.81	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.872		Crippen Method
mcvol	146.770	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
tb	540.17	K	Joback Method
tc	733.44	K	Joback Method
tf	294.56	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.04	J/mol×K	540.17	Joback Method
cpg	384.19	J/mol×K	572.38	Joback Method
cpg	399.44	J/mol×K	604.59	Joback Method
cpg	413.87	J/mol×K	636.80	Joback Method
cpg	427.58	J/mol×K	669.02	Joback Method
cpg	440.64	J/mol×K	701.23	Joback Method

cpg	453.14	J/mol×K	733.44	Joback Method
hvapt	55.70	kJ/mol	421.50	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5445307&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
hvapt:	Enthalpy of vaporization at a given temperature
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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