1-Butylcyclopentanol

Inchi: InChI=1S/C9H18O/c1-2-3-6-9(10)7-4-5-8-9/h10H,2-8H2,1H3
InchiKey: GQTUSXZITATQAM-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CCCCC1(O)CCCC1
Mol. weight [g/mol]: 142.24
CAS: 1462-97-1

Physical Properties

Property code	Value	Unit	Source
gf	-80.86	kJ/mol	Joback Method
hf	-305.60	kJ/mol	Joback Method
hfus	10.79	kJ/mol	Joback Method
hvap	51.41	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.482		Crippen Method
mcvol	132.680	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
tb	465.40 ± 1.50	K	NIST Webbook
tc	702.07	K	Joback Method
tf	286.81	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.41	J/mol×K	513.02	Joback Method
cpg	335.08	J/mol×K	544.53	Joback Method
cpg	348.89	J/mol×K	576.04	Joback Method
cpg	361.93	J/mol×K	607.55	Joback Method
cpg	374.27	J/mol×K	639.05	Joback Method
cpg	386.01	J/mol×K	670.56	Joback Method
cpg	397.22	J/mol×K	702.07	Joback Method
hvapt	63.50	kJ/mol	412.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1462971&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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