N-Butyl-«alpha»-methylbenzylamine

Other names: N-butyl-1-phenylethylamine
Inchi: InChI=1S/C12H19N/c1-3-4-10-13-11(2)12-8-6-5-7-9-12/h5-9,11,13H,3-4,10H2,1-2H3
InchiKey: SHHMVRIBSOJMCK-UHFFFAOYSA-N
Formula: C12H19N
SMILES: CCCCNC(C)c1ccccc1
Mol. weight [g/mol]: 177.29
CAS: 5412-64-6

Physical Properties

Property code	Value	Unit	Source
gf	249.52	kJ/mol	Joback Method
hf	-6.29	kJ/mol	Joback Method
hfus	22.45	kJ/mol	Joback Method
hvap	50.63	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.137		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1307.90		NIST Webbook
tb	550.37	K	Joback Method
tc	755.01	K	Joback Method
tf	289.08	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.67	J/mol×K	550.37	Joback Method
cpg	415.74	J/mol×K	584.48	Joback Method
cpg	431.83	J/mol×K	618.58	Joback Method
cpg	446.99	J/mol×K	652.69	Joback Method
cpg	461.26	J/mol×K	686.80	Joback Method
cpg	474.67	J/mol×K	720.91	Joback Method
cpg	487.26	J/mol×K	755.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5412646&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume