

Benzamide, N-butyl-2-(methylamino)-

Other names:	N-Butyl-2-(methylamino)benzamide
Inchi:	InChI=1S/C12H18N2O/c1-3-4-9-14-12(15)10-7-5-6-8-11(10)13-2/h5-8,13H,3-4,9H2,1-2H
InchiKey:	ZPUCFROBIBAQQV-UHFFFAOYSA-N
Formula:	C12H18N2O
SMILES:	CCCCN=C(O)c1ccccc1NC
Mol. weight [g/mol]:	206.28
CAS:	53693-72-4

Physical Properties

Property code	Value	Unit	Source
hf	-92.28	kJ/mol	Joback Method
hvap	71.75	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.833		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	1830.10		NIST Webbook
rinpol	1830.10		NIST Webbook
tb	724.53	K	Joback Method
tc	930.52	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53693724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemed.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

hf:	Enthalpy of formation at standard conditions
hvac:	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
rinqol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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