

Benzamide, 4-butyl-N-butyl-

Inchi:	InChI=1S/C15H23NO/c1-3-5-7-13-8-10-14(11-9-13)15(17)16-12-6-4-2/h8-11H,3-7,12H2,
InchiKey:	BNJUOUNOHPYPH-UHFFFAOYSA-N
Formula:	C15H23NO
SMILES:	CCCCNC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]:	233.35

Physical Properties

Property code	Value	Unit	Source
gf	138.67	kJ/mol	Joback Method
hf	-186.98	kJ/mol	Joback Method
hfus	34.96	kJ/mol	Joback Method
hvap	65.10	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.559		Crippen Method
mvol	210.000	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	2092.00		NIST Webbook
rinpol	2092.00		NIST Webbook
tb	678.30	K	Joback Method
tc	878.78	K	Joback Method
tf	400.34	K	Joback Method
vc	0.808	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.90	J/molxK	678.30	Joback Method
cpg	591.31	J/molxK	711.71	Joback Method
cpg	606.78	J/molxK	745.13	Joback Method
cpg	621.33	J/molxK	778.54	Joback Method
cpg	635.01	J/molxK	811.96	Joback Method
cpg	647.86	J/molxK	845.37	Joback Method
cpg	659.91	J/molxK	878.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407448&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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