

Benzamide, N,N-dibutyl-4-butyl-

Inchi:	InChI=1S/C19H31NO/c1-4-7-10-17-11-13-18(14-12-17)19(21)20(15-8-5-2)16-9-6-3/h11-
InchiKey:	TUIACEGHXTYPTQ-UHFFFAOYSA-N
Formula:	C19H31NO
SMILES:	CCCCc1ccc(C(=O)N(CCCC)CCCC)cc1
Mol. weight [g/mol]:	289.46

Physical Properties

Property code	Value	Unit	Source
gf	193.74	kJ/mol	Joback Method
hf	-255.48	kJ/mol	Joback Method
hfus	43.24	kJ/mol	Joback Method
hvap	69.62	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.072		Crippen Method
mvol	266.360	ml/mol	McGowan Method
pc	1408.01	kPa	Joback Method
rinpol	2179.00		NIST Webbook
rinpol	2179.00		NIST Webbook
tb	732.09	K	Joback Method
tc	923.01	K	Joback Method
tf	425.23	K	Joback Method
vc	1.016	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.17	J/mol×K	732.09	Joback Method
cpg	797.57	J/mol×K	763.91	Joback Method
cpg	814.94	J/mol×K	795.73	Joback Method
cpg	831.32	J/mol×K	827.55	Joback Method
cpg	846.77	J/mol×K	859.37	Joback Method
cpg	861.33	J/mol×K	891.19	Joback Method
cpg	875.05	J/mol×K	923.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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