Benzamide, N,N-dibutyl-3-methyl-

Other names: Benzamide, 3-methyl, N,N-dibutyl
Inchi: InChI=1S/C16H25NO/c1-4-6-11-17(12-7-5-2)16(18)15-10-8-9-14(3)13-15/h8-10,13H,4-7
InchiKey: FUSJFDNAAFTNNM-UHFFFAOYSA-N
Formula: C16H25NO
SMILES: CCCCN(CCCC)C(=O)c1cccc(C)c1
Mol. weight [g/mol]: 247.38

Physical Properties

Property code	Value	Unit	Source
gf	168.48	kJ/mol	Joback Method
hf	-193.56	kJ/mol	Joback Method
hfus	35.47	kJ/mol	Joback Method
hvap	62.94	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.037		Crippen Method
mcvol	224.090	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	1879.00		NIST Webbook
rinpol	1879.00		NIST Webbook
tb	663.45	K	Joback Method
tc	858.84	K	Joback Method
tf	391.42	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.80	J/mol×K	663.45	Joback Method
cpg	628.39	J/mol×K	696.01	Joback Method
cpg	644.98	J/mol×K	728.58	Joback Method
cpg	660.62	J/mol×K	761.14	Joback Method
cpg	675.35	J/mol×K	793.71	Joback Method
cpg	689.21	J/mol×K	826.27	Joback Method
cpg	702.24	J/mol×K	858.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308554&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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