

Benzamide, 4-butyl-N-butyl-N-2-ethylhexyl-

Inchi:	InChI=1S/C23H39NO/c1-5-9-12-20(8-4)19-24(18-11-7-3)23(25)22-16-14-21(15-17-22)13
InchiKey:	WEQLBBOBVUWVSA-UHFFFAOYSA-N
Formula:	C23H39NO
SMILES:	CCCCc1ccc(C(=O)N(CCCC)CC(CC)CCCC)cc1
Mol. weight [g/mol]:	345.56

Physical Properties

Property code	Value	Unit	Source
gf	224.98	kJ/mol	Joback Method
hf	-343.32	kJ/mol	Joback Method
hfus	50.07	kJ/mol	Joback Method
hvap	78.13	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	6.488		Crippen Method
mvol	322.720	ml/mol	McGowan Method
pc	1081.35	kPa	Joback Method
rinpol	3069.00		NIST Webbook
rinpol	3069.00		NIST Webbook
tb	823.17	K	Joback Method
tc	1016.89	K	Joback Method
tf	455.31	K	Joback Method
vc	1.234	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1018.14	J/molxK	823.17	Joback Method
cpg	1037.64	J/molxK	855.46	Joback Method
cpg	1056.02	J/molxK	887.74	Joback Method
cpg	1073.32	J/molxK	920.03	Joback Method
cpg	1089.61	J/molxK	952.32	Joback Method
cpg	1104.95	J/molxK	984.60	Joback Method
cpg	1119.39	J/molxK	1016.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U415878&Units=SI

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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