

Benzamide, 4-methyl-N-butyl-N-hexyl-

Inchi:	InChI=1S/C18H29NO/c1-4-6-8-9-15-19(14-7-5-2)18(20)17-12-10-16(3)11-13-17/h10-13H
InchiKey:	JCVUBWQZOHZSAC-UHFFFAOYSA-N
Formula:	C18H29NO
SMILES:	CCCCCN(CCCC)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	275.43

Physical Properties

Property code	Value	Unit	Source
gf	185.32	kJ/mol	Joback Method
hf	-234.84	kJ/mol	Joback Method
hfus	40.65	kJ/mol	Joback Method
hvap	67.39	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.818		Crippen Method
mcvol	252.270	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinsol	2894.00		NIST Webbook
rinsol	2894.00		NIST Webbook
tb	709.21	K	Joback Method
tc	901.18	K	Joback Method
tf	413.96	K	Joback Method
vc	0.960	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.93	J/molxK	709.21	Joback Method
cpg	740.08	J/molxK	741.20	Joback Method
cpg	757.22	J/molxK	773.20	Joback Method
cpg	773.38	J/molxK	805.19	Joback Method
cpg	788.62	J/molxK	837.19	Joback Method
cpg	802.97	J/molxK	869.18	Joback Method
cpg	816.49	J/molxK	901.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415925&Units=SI
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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