

Benzamide, 4-methoxy-N-butyl-N-hexyl-

Inchi:	InChI=1S/C18H29NO2/c1-4-6-8-9-15-19(14-7-5-2)18(20)16-10-12-17(21-3)13-11-16/h10
InchiKey:	RTBYFGQCKUOALB-UHFFFAOYSA-N
Formula:	C18H29NO2
SMILES:	CCCCCN(CCCC)C(=O)c1ccc(OC)cc1
Mol. weight [g/mol]:	291.43

Physical Properties

Property code	Value	Unit	Source
gf	80.32	kJ/mol	Joback Method
hf	-367.06	kJ/mol	Joback Method
hfus	41.84	kJ/mol	Joback Method
hvap	69.80	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.518		Crippen Method
mvol	258.140	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpol	2849.00		NIST Webbook
rinpol	2849.00		NIST Webbook
tb	731.63	K	Joback Method
tc	923.19	K	Joback Method
tf	436.19	K	Joback Method
vc	0.978	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.98	J/molxK	731.63	Joback Method
cpg	769.72	J/molxK	763.56	Joback Method
cpg	786.46	J/molxK	795.48	Joback Method
cpg	802.22	J/molxK	827.41	Joback Method
cpg	817.03	J/molxK	859.34	Joback Method
cpg	830.94	J/molxK	891.26	Joback Method
cpg	843.97	J/molxK	923.19	Joback Method

Sources

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=U415909&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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