

Benzamide, 3-methoxy-N-nonyl-

Inchi:	InChI=1S/C17H27NO2/c1-3-4-5-6-7-8-9-13-18-17(19)15-11-10-12-16(14-15)20-2/h10-12
InchiKey:	NZPAWIPVKKHPDY-UHFFFAOYSA-N
Formula:	C17H27NO2
SMILES:	CCCCCCCCNC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	277.40

Physical Properties

Property code	Value	Unit	Source
gf	50.51	kJ/mol	Joback Method
hf	-360.48	kJ/mol	Joback Method
hfus	41.32	kJ/mol	Joback Method
hvap	71.97	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.176		Crippen Method
mvol	244.050	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	2436.00		NIST Webbook
rinpol	2436.00		NIST Webbook
tb	746.48	K	Joback Method
tc	942.49	K	Joback Method
tf	445.11	K	Joback Method
vc	0.939	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.05	J/molxK	746.48	Joback Method
cpg	730.74	J/molxK	779.15	Joback Method
cpg	746.44	J/molxK	811.82	Joback Method
cpg	761.19	J/molxK	844.48	Joback Method
cpg	775.02	J/molxK	877.15	Joback Method
cpg	787.94	J/molxK	909.82	Joback Method
cpg	800.00	J/molxK	942.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407517&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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