

Benzamide, N,N-didecyl-3-methoxy-

Inchi:	InChI=1S/C28H49NO2/c1-4-6-8-10-12-14-16-18-23-29(24-19-17-15-13-11-9-7-5-2)28(30
InchiKey:	NCLSNTVLKJGEPG-UHFFFAOYSA-N
Formula:	C28H49NO2
SMILES:	CCCCCCCCCN(CCCCCCCCCC)C(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	431.69

Physical Properties

Property code	Value	Unit	Source
gf	164.52	kJ/mol	Joback Method
hf	-573.46	kJ/mol	Joback Method
hfus	67.74	kJ/mol	Joback Method
hvap	92.06	kJ/mol	Joback Method
log10ws	-9.27		Crippen Method
logp	8.419		Crippen Method
mvol	399.040	ml/mol	McGowan Method
pc	795.28	kPa	Joback Method
rinpol	3321.00		NIST Webbook
rinpol	3321.00		NIST Webbook
tb	960.43	K	Joback Method
tc	1177.42	K	Joback Method
tf	548.89	K	Joback Method
vc	1.538	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1365.06	J/molxK	960.43	Joback Method
cpg	1385.97	J/molxK	996.59	Joback Method
cpg	1405.41	J/molxK	1032.76	Joback Method
cpg	1423.47	J/molxK	1068.92	Joback Method
cpg	1440.23	J/molxK	1105.09	Joback Method
cpg	1455.77	J/molxK	1141.25	Joback Method
cpg	1470.19	J/molxK	1177.42	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=U308156&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
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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