

Benzamide, N,N-diundecyl-3-methoxy-

Inchi:	InChI=1S/C30H53NO2/c1-4-6-8-10-12-14-16-18-20-25-31(26-21-19-17-15-13-11-9-7-5-2
InchiKey:	FSQZVLAILXHDOE-UHFFFAOYSA-N
Formula:	C30H53NO2
SMILES:	CCCCCCCCCCCN(CCCCCCCCCC)C(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	459.75

Physical Properties

Property code	Value	Unit	Source
gf	181.36	kJ/mol	Joback Method
hf	-614.74	kJ/mol	Joback Method
hfus	72.92	kJ/mol	Joback Method
hvap	96.51	kJ/mol	Joback Method
log10ws	-10.11		Crippen Method
logp	9.199		Crippen Method
mcvol	427.220	ml/mol	McGowan Method
pc	715.68	kPa	Joback Method
tb	1006.19	K	Joback Method
tc	1239.49	K	Joback Method
tf	571.43	K	Joback Method
vc	1.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1494.72	J/molxK	1006.19	Joback Method
cpg	1516.79	J/molxK	1045.07	Joback Method
cpg	1537.20	J/molxK	1083.96	Joback Method
cpg	1556.05	J/molxK	1122.84	Joback Method
cpg	1573.45	J/molxK	1161.72	Joback Method
cpg	1589.53	J/molxK	1200.60	Joback Method
cpg	1604.39	J/molxK	1239.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308157&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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