

Benzamide, N,N-diundecyl-4-methyl-

Inchi:	InChI=1S/C30H53NO/c1-4-6-8-10-12-14-16-18-20-26-31(30(32)29-24-22-28(3)23-25-29)
InchiKey:	NAXZIGNVXWOYPO-UHFFFAOYSA-N
Formula:	C30H53NO
SMILES:	CCCCCCCCCN(CCCCCCCCCC)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	443.75

Physical Properties

Property code	Value	Unit	Source
gf	286.36	kJ/mol	Joback Method
hf	-482.52	kJ/mol	Joback Method
hfus	71.73	kJ/mol	Joback Method
hvap	94.10	kJ/mol	Joback Method
log10ws	-10.46		Crippen Method
logp	9.499		Crippen Method
mvol	421.350	ml/mol	McGowan Method
pc	722.24	kPa	Joback Method
rinpol	3507.00		NIST Webbook
rinpol	3507.00		NIST Webbook
tb	983.77	K	Joback Method
tc	1208.74	K	Joback Method
tf	549.20	K	Joback Method
vc	1.631	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.61	J/molxK	983.77	Joback Method
cpg	1485.12	J/molxK	1021.27	Joback Method
cpg	1506.18	J/molxK	1058.76	Joback Method
cpg	1525.91	J/molxK	1096.26	Joback Method
cpg	1544.41	J/molxK	1133.75	Joback Method
cpg	1561.81	J/molxK	1171.25	Joback Method
cpg	1578.23	J/molxK	1208.74	Joback Method

Sources

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=U308470&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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