

Benzamide, N-cyclohexyl-N-[(cyclohexylamino)carbonyl]-

Other names:

N-Benzoyl-N,N'-dicyclohexylurea

Urea, 1-benzoyl-1,3-dicyclohexyl-

Inchi: InChI=1S/C20H28N2O2/c23-19(16-10-4-1-5-11-16)22(18-14-8-3-9-15-18)20(24)21-17-12

InchiKey: OXHQJTMLYJFMCW-UHFFFAOYSA-N

Formula: C20H28N2O2

SMILES: O=C(NC1CCCCC1)N(C(=O)c1cccc1)C1CCCCC1

Mol. weight [g/mol]: 328.45

CAS: 3080-42-0

Physical Properties

Property code	Value	Unit	Source
gf	221.16	kJ/mol	Joback Method
hf	-215.12	kJ/mol	Joback Method
hfus	36.58	kJ/mol	Joback Method
hvap	85.22	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	4.504		Crippen Method
mvol	270.280	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
tb	893.13	K	Joback Method
tc	1138.82	K	Joback Method
tf	541.33	K	Joback Method
vc	0.979	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.00	J/molxK	893.13	Joback Method
cpg	930.18	J/molxK	934.08	Joback Method
cpg	946.57	J/molxK	975.03	Joback Method
cpg	961.28	J/molxK	1015.97	Joback Method
cpg	974.43	J/molxK	1056.92	Joback Method
cpg	986.16	J/molxK	1097.87	Joback Method
cpg	996.59	J/molxK	1138.82	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=C3080420&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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