N-BENZOYL-N,N'-DICYCLOHEXYLUREA

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)c1ccccc1)C1CCCCC1
Mol. weight [g/mol]: 328.46

Physical Properties

Property code	Value	Unit	Source
hfus	36.59	kJ/mol	Joback Method
log10ws	-4.47		Cheméo Relay (1.0)
logp	4.504		Crippen Method
mcvol	270.280	ml/mol	McGowan Method
tb	668.10	K	Cheméo Relay (1.0)
tf	378.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.00	J/mol×K	893.13	Joback Method
cpg	930.18	J/mol×K	934.08	Joback Method
cpg	946.57	J/mol×K	975.03	Joback Method
cpg	961.28	J/mol×K	1015.97	Joback Method
cpg	974.43	J/mol×K	1056.92	Joback Method
cpg	986.16	J/mol×K	1097.87	Joback Method
cpg	996.59	J/mol×K	1138.82	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3080420&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point