

Benzamide, N,N-dibenzoyl-

Inchi:	InChI=1S/C21H15NO3/c23-19(16-10-4-1-5-11-16)22(20(24)17-12-6-2-7-13-17)21(25)18-
InchiKey:	UVUKMPQRNIREDM-UHFFFAOYSA-N
Formula:	C21H15NO3
SMILES:	O=C(c1ccccc1)N(C(=O)c1ccccc1)C(=O)c1ccccc1
Mol. weight [g/mol]:	329.35
CAS:	602-88-0

Physical Properties

Property code	Value	Unit	Source
chs	-10112.60	kJ/mol	NIST Webbook
gf	187.19	kJ/mol	Joback Method
hf	-37.39	kJ/mol	Joback Method
hfus	40.09	kJ/mol	Joback Method
hvap	91.45	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	3.810		Crippen Method
mcvol	250.160	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
tb	933.97	K	Joback Method
tc	1193.84	K	Joback Method
tf	587.95	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.97	J/molxK	933.97	Joback Method
cpg	746.62	J/molxK	977.28	Joback Method
cpg	757.09	J/molxK	1020.59	Joback Method
cpg	766.55	J/molxK	1063.91	Joback Method
cpg	775.14	J/molxK	1107.22	Joback Method
cpg	783.02	J/molxK	1150.53	Joback Method
cpg	790.36	J/molxK	1193.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C602880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

chs:	Standard solid enthalpy of combustion
cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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