N-Benzoyl-o-aminodiphenylamine

Inchi: InChI=1S/C19H16N2O/c22-19(15-9-3-1-4-10-15)21-18-14-8-7-13-17(18)20-16-11-5-2-6-
InchiKey: UZFYPOXSNSAIKK-UHFFFAOYSA-N
Formula: C19H16N2O
SMILES: O=C(Nc1ccccc1Nc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 288.34
CAS: 34237-88-2

Physical Properties

Property code	Value	Unit	Source
chs	-9753.00 ± 84.00	kJ/mol	NIST Webbook
gf	486.56	kJ/mol	Joback Method
hf	256.99	kJ/mol	Joback Method
hfs	-10.00 ± 84.00	kJ/mol	NIST Webbook
hfus	38.50	kJ/mol	Joback Method
hvap	85.00	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.683		Crippen Method
mcvol	228.820	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
ss	340.70	J/mol×K	NIST Webbook
tb	873.35	K	Joback Method
tc	1132.42	K	Joback Method
tf	550.92	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.96	J/mol×K	873.35	Joback Method
cpg	681.38	J/mol×K	916.53	Joback Method
cpg	693.49	J/mol×K	959.71	Joback Method
cpg	704.44	J/mol×K	1002.89	Joback Method
cpg	714.35	J/mol×K	1046.06	Joback Method
cpg	723.37	J/mol×K	1089.24	Joback Method

cpg	731.62	J/mol×K	1132.42	Joback Method
cps	356.60	J/mol×K	298.15	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34237882&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume