1-Butanone, 3,3'-(1,2-ethanediyldinitrilo)bis[1-phenyl-

Other names: Butyrophenone, 3,3''-(ethylenedinitrilo)di-
3-[(2-([1-Methyl-3-oxo-3-phenylpropylidene]amino)ethyl)imino]-1-phenyl-1-butanone
N,N'-Ethylenebis(3-amino-1-phenyl-but-2-en-1-one)

Inchi: InChI=1S/C22H24N2O2/c1-17(15-21(25)19-9-5-3-6-10-19)23-13-14-24-18(2)16-22(26)20

InchiKey: CODOLTFDVSRVJU-UHFFFAOYSA-N

Formula: C22H24N2O2

SMILES: CC(CC(=O)c1ccccc1)=NCCN=C(C)CC(=O)c1ccccc1

Mol. weight [g/mol]: 348.44

CAS: 16087-30-2

Physical Properties

Property code	Value	Unit	Source
chs	-11783.90 ± 4.20	kJ/mol	NIST Webbook
hf	-104.50 ± 7.50	kJ/mol	NIST Webbook
hfs	-303.30 ± 5.10	kJ/mol	NIST Webbook
hsub	198.80 ± 5.30	kJ/mol	NIST Webbook
hsub	198.80 ± 5.30	kJ/mol	NIST Webbook
hvap	89.40	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.454		Crippen Method
mcvol	287.820	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
tb	1016.98	K	Joback Method
tc	1266.55	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	192.90 ± 5.30	kJ/mol	416.50	NIST Webbook

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=C16087302&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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