

Ethanediamide, N,N'-bis(phenylmethyl)-

Other names:	N,N'-Dibenzoyloxamide
Inchi:	InChI=1S/C16H16N2O2/c19-15(17-11-13-7-3-1-4-8-13)16(20)18-12-14-9-5-2-6-10-14/h1
InchiKey:	AOIKOYRULAZZLJ-UHFFFAOYSA-N
Formula:	C16H16N2O2
SMILES:	O=C(NCc1ccccc1)C(=O)NCc1ccccc1
Mol. weight [g/mol]:	268.31
CAS:	3551-78-8

Physical Properties

Property code	Value	Unit	Source
gf	229.60	kJ/mol	Joback Method
hf	-18.73	kJ/mol	Joback Method
hfus	38.67	kJ/mol	Joback Method
hvap	82.13	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	1.619		Crippen Method
mcvol	211.880	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	2467.10		NIST Webbook
rinpol	2467.10		NIST Webbook
tb	826.92	K	Joback Method
tc	1064.02	K	Joback Method
tf	528.10	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.47	J/molxK	826.92	Joback Method
cpg	624.25	J/molxK	866.44	Joback Method
cpg	635.89	J/molxK	905.95	Joback Method
cpg	646.49	J/molxK	945.47	Joback Method
cpg	656.13	J/molxK	984.99	Joback Method
cpg	664.89	J/molxK	1024.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3551788&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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