

2'-PHENYLACETANILIDE

Other names:	2'-Phenylacetanilide 2-Acetamido-diphenyl 2-Acetamidobiphenyl 2-Acetylaminobiphenyl Acetanilide, 2'-phenyl- Acetanilide, o-phenyl- N-(2-(Phenyl)phenyl)acetamide N-(2-Biphenyl)acetamide N-[2-Biphenyl]acetamide NSC 3158 NSC 50998
Inchi:	InChI=1S/C14H13NO/c1-11(16)15-14-10-6-5-9-13(14)12-7-3-2-4-8-12/h2-10H,1H3,(H,15
InchiKey:	IXCZSZXIGHWLEJ-UHFFFAOYSA-N
Formula:	C14H13NO
SMILES:	CC(=O)Nc1ccccc1-c1ccccc1
Mol. weight [g/mol]:	211.26

Physical Properties

Property code	Value	Unit	Source
af	0.5688		Cheméo Relay (1.0)
hf	-21.09	kJ/mol	Cheméo Relay (1.0)
hfus	26.41	kJ/mol	Joback Method
hvap	92.46	kJ/mol	Cheméo Relay (1.0)
ie	7.94	eV	Cheméo Relay (1.0)
log10ws	-3.19		Cheméo Relay (1.0)
logp	3.312		Crippen Method
mcvol	172.150	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
tb	615.80	K	Cheméo Relay (1.0)
tc	901.49	K	Cheméo Relay (1.0)
tf	360.71	K	Cheméo Relay (1.0)
vc	0.617	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.30	J/mol×K	682.10	Joback Method
cpg	455.12	J/mol×K	722.87	Joback Method
cpg	468.73	J/mol×K	763.64	Joback Method
cpg	481.19	J/mol×K	804.41	Joback Method
cpg	492.58	J/mol×K	845.18	Joback Method
cpg	502.98	J/mol×K	885.95	Joback Method
cpg	512.46	J/mol×K	926.72	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2113475&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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):

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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