

N-acetyl-carbazole

Inchi:	InChI=1S/C14H11NO/c1-10(16)15-13-8-4-2-6-11(13)12-7-3-5-9-14(12)15/h2-9H,1H3
InchiKey:	CADSTRJVECIAT-UHFFFAOYSA-N
Formula:	C14H11NO
SMILES:	CC(=O)n1c2ccccc2c2ccccc21
Mol. weight [g/mol]:	209.24
CAS:	574-39-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.20		Crippen Method
logp	3.455		Crippen Method
mcvol	161.290	ml/mol	McGowan Method
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
ripol	3214.00		NIST Webbook
ripol	3214.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	15.10	kJ/mol	349.90	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C574390&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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