

N-acetyl-di-p-tolylamine

Inchi:	InChI=1S/C16H17NO/c1-12-4-8-15(9-5-12)17(14(3)18)16-10-6-13(2)7-11-16/h4-11H,1-3
InchiKey:	PFVHRXRSOITNHZ-UHFFFAOYSA-N
Formula:	C16H17NO
SMILES:	CC(=O)N(c1ccc(C)cc1)c1ccc(C)cc1
Mol. weight [g/mol]:	239.31
CAS:	32047-89-5

Physical Properties

Property code	Value	Unit	Source
gf	271.26	kJ/mol	Joback Method
hf	31.50	kJ/mol	Joback Method
hfus	29.12	kJ/mol	Joback Method
hvap	65.88	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.988		Crippen Method
mcvol	200.330	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
tb	695.11	K	Joback Method
tc	929.42	K	Joback Method
tf	430.36	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.62	J/molxK	695.11	Joback Method
cpg	546.07	J/molxK	734.16	Joback Method
cpg	561.27	J/molxK	773.21	Joback Method
cpg	575.29	J/molxK	812.26	Joback Method
cpg	588.22	J/molxK	851.31	Joback Method
cpg	600.12	J/molxK	890.36	Joback Method
cpg	611.07	J/molxK	929.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32047895&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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