Di-p-tolylamine, N-acetyl-

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]: 239.32

Physical Properties

Property code	Value	Unit	Source
af	0.6515		Cheméo Relay (1.0)
gf	271.26	kJ/mol	Joback Method
hf	-43.77	kJ/mol	Cheméo Relay (1.0)
hfus	29.12	kJ/mol	Joback Method
hvap	84.68	kJ/mol	Cheméo Relay (1.0)
ie	7.73	eV	Cheméo Relay (1.0)
log10ws	-4.12		Cheméo Relay (1.0)
logp	3.988		Crippen Method
mcvol	200.330	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
tb	624.35	K	Cheméo Relay (1.0)
tc	898.13	K	Cheméo Relay (1.0)
tf	389.22	K	Cheméo Relay (1.0)
vc	0.730	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32047895&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):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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