Di-o-tolyl-cyano-methane

Inchi: InChI=1S/C16H15N/c1-12-7-3-5-9-14(12)16(11-17)15-10-6-4-8-13(15)2/h3-10,16H,1-2H3
InchiKey: KDKUNNHFMPKKTB-UHFFFAOYSA-N
Formula: C16H15N
SMILES: Cc1ccccc1C(C#N)c1ccccc1C
Mol. weight [g/mol]: 221.30
CAS: 116296-33-4

Physical Properties

Property code	Value	Unit	Source
gf	420.14	kJ/mol	Joback Method
hf	236.15	kJ/mol	Joback Method
hfus	22.48	kJ/mol	Joback Method
hvap	67.18	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.959		Crippen Method
mcvol	190.160	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
tb	730.44	K	Joback Method
tc	978.73	K	Joback Method
tf	397.95	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.06	J/mol×K	730.44	Joback Method
cpg	515.93	J/mol×K	771.82	Joback Method
cpg	529.61	J/mol×K	813.20	Joback Method
cpg	542.19	J/mol×K	854.58	Joback Method
cpg	553.73	J/mol×K	895.97	Joback Method
cpg	564.31	J/mol×K	937.35	Joback Method
cpg	574.01	J/mol×K	978.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116296334&Units=SI

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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