Benzene, 1-dimethylamino-4-(2-cyano-2-phenylethenyl)

Inchi: InChI=1S/C17H16N2/c1-19(2)17-10-8-14(9-11-17)12-16(13-18)15-6-4-3-5-7-15/h3-12H,1

InchiKey: HYAJIHDALOHMPT-FOWTUZBSSA-N

Formula: C17H16N2

SMILES: CN(C)c1ccc(C=C(C#N)c2ccccc2)cc1

Mol. weight [g/mol]: 248.32

CAS: 1222-61-3

Physical Properties

Property code	Value	Unit	Source
chs	-9084.00	kJ/mol	NIST Webbook
chs	-9079.00	kJ/mol	NIST Webbook
gf	623.08	kJ/mol	Joback Method
hf	407.22	kJ/mol	Joback Method
hfs	104.00	kJ/mol	NIST Webbook
hfs	103.00	kJ/mol	NIST Webbook
hfus	30.90	kJ/mol	Joback Method
hvap	71.21	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.817		Crippen Method
mcvol	209.930	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
tb	765.26	K	Joback Method
tc	1012.19	K	Joback Method
tf	425.13	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.24	J/mol×K	765.26	Joback Method
cpg	584.02	J/mol×K	806.41	Joback Method
cpg	597.63	J/mol×K	847.57	Joback Method
cpg	610.20	J/mol×K	888.72	Joback Method
cpg	621.85	J/mol×K	929.88	Joback Method

cpg	632.71	J/mol×K	971.03	Joback Method
cpg	642.90	J/mol×K	1012.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1222613&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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