BENZENE, 1-DIMETHYLAMINO-4(2-CYANO-2-PHENYLETHEN

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]: 248.33

Physical Properties

Property code	Value	Unit	Source
af	0.6048		Cheméo Relay (1.0)
gf	623.08	kJ/mol	Joback Method
hf	377.85	kJ/mol	Cheméo Relay (1.0)
hfus	30.90	kJ/mol	Joback Method
ie	7.34	eV	Cheméo Relay (1.0)
log10ws	-4.79		Cheméo Relay (1.0)
logp	3.817		Crippen Method
mcvol	209.930	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
tb	663.92	K	Cheméo Relay (1.0)
tc	921.07	K	Cheméo Relay (1.0)
tf	387.09	K	Cheméo Relay (1.0)

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

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1222613&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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