Benzene, 1-dimethylamino-4-(2,2-dicyanoethenyl)

Other names: p-N,N-Dimethylaminobenzal malononitrile
(4-Dimethylaminobenzyliden)-malodinitril
(4-Dimethylaminobenzylidene)malodinitrile

Inchi: InChI=1S/C12H11N3/c1-15(2)12-5-3-10(4-6-12)7-11(8-13)9-14/h3-7H,1-2H3

InchiKey: IYNONQVNLZATDK-UHFFFAOYSA-N

Formula: C12H11N3

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

Mol. weight [g/mol]: 197.24

CAS: 2826-28-0

Physical Properties

Property code	Value	Unit	Source
gf	601.75	kJ/mol	Joback Method
hf	438.77	kJ/mol	Joback Method
hfus	25.41	kJ/mol	Joback Method
hvap	68.28	kJ/mol	Joback Method
ie	7.80	eV	NIST Webbook
ie	7.60	eV	NIST Webbook
log10ws	-2.77		Crippen Method
logp	2.183		Crippen Method
mcvol	164.620	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
tb	726.26	K	Joback Method
tc	964.23	K	Joback Method
tf	407.35	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.77	J/mol×K	726.26	Joback Method
cpg	426.65	J/mol×K	765.92	Joback Method
cpg	436.72	J/mol×K	805.58	Joback Method
cpg	446.06	J/mol×K	845.25	Joback Method

cpg	454.75	J/mol×K	884.91	Joback Method
cpg	462.86	J/mol×K	924.57	Joback Method
cpg	470.48	J/mol×K	964.23	Joback Method

Sources

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=C2826280&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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