

Terephthalonitrile N,N'-dioxide

Other names:	1,4-Dicyanobenzene di-N-oxide
Inchi:	InChI=1S/C8H4N2O2/c11-9-5-7-1-2-8(4-3-7)6-10-12/h1-4H
InchiKey:	JRVRIUGIFUNROE-UHFFFAOYSA-N
Formula:	C8H4N2O2
SMILES:	[O-][N+]#Cc1ccc(C#[N+][O-])cc1
Mol. weight [g/mol]:	160.13
CAS:	3729-34-8

Physical Properties

Property code	Value	Unit	Source
chs	-4057.20 ± 1.50	kJ/mol	NIST Webbook
hf	410.50 ± 2.70	kJ/mol	NIST Webbook
hfs	337.50 ± 1.80	kJ/mol	NIST Webbook
hsub	73.00 ± 2.00	kJ/mol	NIST Webbook
hsub	73.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-8.88		Crippen Method
logp	2.044		Crippen Method
mcvol	114.320	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3729348&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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