Tetracyano-p-quinodimethane

Other names:	Propanedinitrile, 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis-
	2,5-Cyclohexadiene-«delta»1,«alpha»:4,«alpha»'-dimalononitrile
	Quinodimethan, tetracyano-
	Tetracyanoquinodimethan(e)
	TCNQ
	2,5-Cyclohexadiene-1,4-Diylidenedimalononitrile
	7,7,8,8-Tetracyano-p-quinodimethane
	7,7,8,8-Tetracyano-1,4-quinodimethan
	7,7,8,8-Tetracyanoquinodimethane
	7,7',8,8'-Tetracyanoquinodimethane
	2,5-Cyclohexadiene-1,4-diylidene-«alpha»,«alpha»'-dimalononitrile
	Tetracyanoquinodimethan
	NSC 105237
	2,2'-(2,5-cyclohexadiene-1,4-diylidene)bismalononitrile
Inchi:	InChI=1S/C12H4N4/c13-5-11(6-14)9-1-2-10(4-3-9)12(7-15)8-16/h1-4H
InchiKey:	PCCVSPMFGIFTHU-UHFFFAOYSA-N
Formula:	C12H4N4
SMILES:	N#CC(C#N)=c1ccc(=C(C#N)C#N)cc1
Mol. weight [g/mol]:	204.19
CAS:	1518-16-7

Physical Properties

Property code	Value	Unit	Source
chs	-5959.00 ± 3.00	kJ/mol	NIST Webbook
chs	-5958.90 ± 5.70	kJ/mol	NIST Webbook
ea	2.80 ± 0.10	eV	NIST Webbook
ea	2.88 ± 0.19	eV	NIST Webbook
ea	2.80 ± 0.10	eV	NIST Webbook
ea	2.80 ± 0.30	eV	NIST Webbook
hf	771.10	kJ/mol	NIST Webbook
hf	770.00 ± 10.00	kJ/mol	NIST Webbook
hfs	665.00 ± 3.00	kJ/mol	NIST Webbook
hfs	666.10 ± 5.90	kJ/mol	NIST Webbook
hsub	105.00	kJ/mol	NIST Webbook
hsub	105.00	kJ/mol	NIST Webbook
log10ws	-2.07		Crippen Method
logp	0.082		Crippen Method

mcvol	157.400	ml/mol	McGowan Method
tf	567.00 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	108.00 ± 2.00	kJ/mol	502.50	NIST Webbook
hsubt	122.00 ± 2.00	kJ/mol	423.00	NIST Webbook
hsubt	126.00 ± 1.00	kJ/mol	413.00	NIST Webbook
hsubt	105.00 ± 10.00	kJ/mol	466.00	NIST Webbook
hsubt	105.00 ± 9.20	kJ/mol	465.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1518167&Units=SI

Legend

chs: Standard solid enthalpy of combustion
ea: Electron affinity
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.