

NITROBENZENE, 3-(2,2-DICYANOETHENYL)

Other names:	(3-Nitrobenzylidene)malononitrile m-Nitrobenzylidenemalononitrile Malononitrile, (m-nitrobenzylidene)- Propanedinitrile, ((3-nitrophenyl)methylene)-
Inchi:	InChI=1S/C10H5N3O2/c11-6-9(7-12)4-8-2-1-3-10(5-8)13(14)15/h1-5H
InchiKey:	UQMJZLGIKHAOQZ-UHFFFAOYSA-N
Formula:	C10H5N3O2
SMILES:	N#CC(C#N)=Cc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	199.17

Physical Properties

Property code	Value	Unit	Source
hf	445.03	kJ/mol	Cheméo Relay (1.0)
hfus	28.57	kJ/mol	Joback Method
hvap	79.28	kJ/mol	Cheméo Relay (1.0)
ie	9.93	eV	Cheméo Relay (1.0)
log10ws	-3.25		Cheméo Relay (1.0)
logp	2.025		Crippen Method
mcvol	143.880	ml/mol	McGowan Method
tb	577.52	K	Cheméo Relay (1.0)
tf	390.08	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.55	J/mol×K	819.90	Joback Method
cpg	363.03	J/mol×K	864.85	Joback Method
cpg	369.87	J/mol×K	909.79	Joback Method
cpg	376.15	J/mol×K	954.74	Joback Method
cpg	381.97	J/mol×K	999.69	Joback Method
cpg	387.42	J/mol×K	1044.63	Joback Method
cpg	392.58	J/mol×K	1089.58	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2826326&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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