Propanedinitrile, (phenylmethylene)-

Other names:	Malononitrile, benzylidene-
	«alpha»-Cyanocinnamonitrile
	«beta»,«beta»-Dicyanostyrene
	Benzalmalononitrile
	Benzylidenemalonodinitrile
	Benzylidenemalononitrile
	2-Phenyl-1,1-dicyanoethylene
	2,2-Dicyano-1-phenylethylene
	Benzalmalonitrile
	BMN
	Benzal-malonitril
	F 2370
	1,1-Dicyano-2-phenylethene
	1,1-Dicyano-2-phenylethylene
	2-Cyano-3-phenylacrylonitrile
	2-Phenyl-1,1-dicyanoethene
	Malonodinitrile, benzylidene
	Benzylidenemalonitrile
	NSC 490
	Propanedinitrile, 2-(phenylmethylene)-
	«beta»,«beta»-Styrenedicarbonitrile
	beta,beta-styrenedicarbonitrile
Inchi:	InChI=1S/C10H6N2/c11-7-10(8-12)6-9-4-2-1-3-5-9/h1-6H
InchiKey:	WAVNYPVYNSIHNC-UHFFFAOYSA-N
Formula:	C10H6N2
SMILES:	N#CC(C#N)=Cc1ccccc1
Mol. weight [g/mol]:	154.17
CAS:	2700-22-3

Physical Properties

Property code	Value	Unit	Source
gf	483.76	kJ/mol	Joback Method
hf	423.99	kJ/mol	Joback Method
hfus	17.60	kJ/mol	Joback Method
hvap	61.12	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method

logp	2.117		Crippen Method
mcvol	126.460	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1487.00		NIST Webbook
tb	663.08	K	Joback Method
tc	914.90	K	Joback Method
tf	339.82	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.38	J/mol×K	663.08	Joback Method
cpg	292.43	J/mol×K	705.05	Joback Method
cpg	300.72	J/mol×K	747.02	Joback Method
cpg	308.32	J/mol×K	788.99	Joback Method
cpg	315.31	J/mol×K	830.96	Joback Method
cpg	321.77	J/mol×K	872.93	Joback Method
cpg	327.76	J/mol×K	914.90	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2700223&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume