

Malononitrile, (diphenylmethylene)-

Other names:	Diphenylmethylenemalononitrile «alpha»-Cyano-«beta», «beta»-diphenylacrylonitrile «alpha»-Phenylbenzalmalononitrile Dicyan Dicyan (antioxidant) Propanedinitrile, (diphenylmethylene)- TsN 2 1,1-Dicyano-2,2-diphenylethylene 1,1-Diphenyl-2,2-dicyanoethylene 1,1-Dicyano-2,2-diphenyl-ethene Benzhydrylidene malononitrile NSC 509569 Malonitrile, diphenylmethylene
Inchi:	InChI=1S/C16H10N2/c17-11-15(12-18)16(13-7-3-1-4-8-13)14-9-5-2-6-10-14/h1-10H
InchiKey:	KOQMBAGMXLUQDS-UHFFFAOYSA-N
Formula:	C16H10N2
SMILES:	N#CC(C#N)=C(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	230.26
CAS:	10394-96-4

Physical Properties

Property code	Value	Unit	Source
gf	638.14	kJ/mol	Joback Method
hf	526.89	kJ/mol	Joback Method
hfus	25.87	kJ/mol	Joback Method
hvap	76.84	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.536		Crippen Method
mcvol	187.240	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
tb	826.92	K	Joback Method
tc	1095.76	K	Joback Method
tf	419.90	K	Joback Method
vc	0.750	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.34	J/mol×K	826.92	Joback Method
cpg	502.45	J/mol×K	871.73	Joback Method
cpg	512.62	J/mol×K	916.53	Joback Method
cpg	522.00	J/mol×K	961.34	Joback Method
cpg	530.74	J/mol×K	1006.15	Joback Method
cpg	538.97	J/mol×K	1050.95	Joback Method
cpg	546.85	J/mol×K	1095.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10394964&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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