Malononitrile, phenyl-

Other names:	Phenyl-malonitril
	Phenylmalononitrile
	Propanedinitrile, phenyl-
	2-Phenylmalononitrile
Inchi:	InChI=1S/C9H6N2/c10-6-9(7-11)8-4-2-1-3-5-8/h1-5,9H
InchiKey:	OFCTVAYVCDCQDA-UHFFFAOYSA-N
Formula:	C9H6N2
SMILES:	N#CC(C#N)c1ccccc1
Mol. weight [g/mol]:	142.16
CAS:	3041-40-5

Physical Properties

Property code	Value	Unit	Source
gf	401.23	kJ/mol	Joback Method
hf	331.92	kJ/mol	Joback Method
hfus	12.60	kJ/mol	Joback Method
hvap	58.47	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	1.817		Crippen Method
mcvol	116.670	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	635.72	K	Joback Method
tc	883.30	K	Joback Method
tf	332.59	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.50	J/mol×K	635.72	Joback Method
cpg	269.59	J/mol×K	676.98	Joback Method
cpg	277.93	J/mol×K	718.25	Joback Method
cpg	285.57	J/mol×K	759.51	Joback Method
cpg	292.57	J/mol×K	800.77	Joback Method

cpg	298.95	J/mol×K	842.04	Joback Method
cpg	304.78	J/mol×K	883.30	Joback Method

Sources

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=C3041405&Units=SI
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
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