1-Phenyl-1,4-dicyano-1,2,3,4-tetrahydronaphthale

Other names: 1-Phenyl-1,2,3,4-tetrahydro-1,4-naphthalenedicarbonitrile
1,4-Naphthalenedinitrile, 1,2,3,4-tetrahydro-4-phenyl-
Inchi: InChI=1S/C18H14N2/c19-12-14-10-11-18(13-20,15-6-2-1-3-7-15)17-9-5-4-8-16(14)17/h1
InchiKey: VPBGDRICPKPSNM-UHFFFAOYSA-N
Formula: C18H14N2
SMILES: N#CC1CCC(C#N)(c2ccccc2)c2ccccc21
Mol. weight [g/mol]: 258.32
CAS: 25679-87-2

Physical Properties

Property code	Value	Unit	Source
gf	617.68	kJ/mol	Joback Method
hf	438.04	kJ/mol	Joback Method
hfus	23.89	kJ/mol	Joback Method
hvap	80.46	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.897		Crippen Method
mcvol	208.860	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
tb	880.32	K	Joback Method
tc	1152.53	K	Joback Method
tf	522.04	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.08	J/mol×K	880.32	Joback Method
cpg	630.03	J/mol×K	925.69	Joback Method
cpg	646.00	J/mol×K	971.06	Joback Method
cpg	662.30	J/mol×K	1016.43	Joback Method
cpg	679.23	J/mol×K	1061.79	Joback Method
cpg	697.11	J/mol×K	1107.16	Joback Method
cpg	716.24	J/mol×K	1152.53	Joback Method

Sources

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=C25679872&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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