3-Methyl-2-phenyl-but-2-enenitrile

Inchi: InChI=1S/C11H11N/c1-9(2)11(8-12)10-6-4-3-5-7-10/h3-7H,1-2H3
InchiKey: IWOSBVMKLPSAAJ-UHFFFAOYSA-N
Formula: C11H11N
SMILES: CC(C)=C(C#N)c1ccccc1
Mol. weight [g/mol]: 157.21
CAS: 18670-23-0

Physical Properties

Property code	Value	Unit	Source
chs	-6097.97	kJ/mol	NIST Webbook
gf	350.45	kJ/mol	Joback Method
hf	228.68	kJ/mol	Joback Method
hfs	197.20	kJ/mol	NIST Webbook
hfus	17.38	kJ/mol	Joback Method
hvap	52.95	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.004		Crippen Method
mcvol	139.170	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
tb	583.76	K	Joback Method
tc	821.58	K	Joback Method
tf	272.14	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.90	J/mol×K	583.76	Joback Method
cpg	327.05	J/mol×K	623.40	Joback Method
cpg	339.22	J/mol×K	663.03	Joback Method
cpg	350.50	J/mol×K	702.67	Joback Method
cpg	360.95	J/mol×K	742.31	Joback Method
cpg	370.65	J/mol×K	781.95	Joback Method
cpg	379.66	J/mol×K	821.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18670230&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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