2-Phenyl-peny-2-enenitrile

Inchi: InChI=1S/C11H11N/c1-2-6-11(9-12)10-7-4-3-5-8-10/h3-8H,2H2,1H3/b11-6+
InchiKey: VSWFBCVGAVHYAX-IZZDOVSWSA-N
Formula: C11H11N
SMILES: CCC=C(C#N)c1ccccc1
Mol. weight [g/mol]: 157.21
CAS: 6519-08-0

Physical Properties

Property code	Value	Unit	Source
chs	-6103.74	kJ/mol	NIST Webbook
gf	359.00	kJ/mol	Joback Method
hf	238.47	kJ/mol	Joback Method
hfs	203.00	kJ/mol	NIST Webbook
hfus	18.68	kJ/mol	Joback Method
hvap	52.87	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.004		Crippen Method
mcvol	139.170	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
tb	583.88	K	Joback Method
tc	817.29	K	Joback Method
tf	286.10	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.11	J/mol×K	583.88	Joback Method
cpg	327.05	J/mol×K	622.78	Joback Method
cpg	339.05	J/mol×K	661.68	Joback Method
cpg	350.18	J/mol×K	700.59	Joback Method
cpg	360.51	J/mol×K	739.49	Joback Method
cpg	370.10	J/mol×K	778.39	Joback Method
cpg	379.03	J/mol×K	817.29	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=C6519080&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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