4-Methyl-2-phenyl-pent-2-enenitrile

Inchi: InChI=1S/C12H13N/c1-10(2)8-12(9-13)11-6-4-3-5-7-11/h3-8,10H,1-2H3/b12-8+
InchiKey: HEMJEFCPWMCERS-XYOKQWHBSA-N
Formula: C12H13N
SMILES: CC(C)C=C(C#N)c1ccccc1
Mol. weight [g/mol]: 171.24
CAS: 6519-10-4

Physical Properties

Property code	Value	Unit	Source
gf	364.98	kJ/mol	Joback Method
hf	212.55	kJ/mol	Joback Method
hfus	17.75	kJ/mol	Joback Method
hvap	54.71	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.250		Crippen Method
mcvol	153.260	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
tb	606.32	K	Joback Method
tc	840.13	K	Joback Method
tf	282.37	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.66	J/mol×K	606.32	Joback Method
cpg	375.71	J/mol×K	645.29	Joback Method
cpg	388.76	J/mol×K	684.26	Joback Method
cpg	400.87	J/mol×K	723.23	Joback Method
cpg	412.11	J/mol×K	762.19	Joback Method
cpg	422.56	J/mol×K	801.16	Joback Method
cpg	432.28	J/mol×K	840.13	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=C6519104&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