5-Methyl-2-phenyl-hex-2-enenitrile

Inchi: InChI=1S/C13H15N/c1-11(2)8-9-13(10-14)12-6-4-3-5-7-12/h3-7,9,11H,8H2,1-2H3/b13-9-
InchiKey: CLDPKOSCBSRXFB-UKTHLTGXSA-N
Formula: C13H15N
SMILES: CC(C)CC=C(C#N)c1ccccc1
Mol. weight [g/mol]: 185.26
CAS: 6519-11-5

Physical Properties

Property code	Value	Unit	Source
chs	-7406.47	kJ/mol	NIST Webbook
gf	373.40	kJ/mol	Joback Method
hf	191.91	kJ/mol	Joback Method
hfs	147.00	kJ/mol	NIST Webbook
hfus	20.34	kJ/mol	Joback Method
hvap	56.94	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.640		Crippen Method
mcvol	167.350	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
tb	629.20	K	Joback Method
tc	858.39	K	Joback Method
tf	293.64	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.33	J/mol×K	629.20	Joback Method
cpg	425.04	J/mol×K	667.40	Joback Method
cpg	438.72	J/mol×K	705.60	Joback Method
cpg	451.46	J/mol×K	743.80	Joback Method
cpg	463.32	J/mol×K	782.00	Joback Method
cpg	474.37	J/mol×K	820.20	Joback Method
cpg	484.68	J/mol×K	858.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6519115&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

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