2-Phenyl-hex-2-enenitrile

Other names: Benzeneacetonitrile, «alpha»-butylidene-
2-Hexenenitrile, 2-phenyl
Inchi: InChI=1S/C12H13N/c1-2-3-7-12(10-13)11-8-5-4-6-9-11/h4-9H,2-3H2,1H3/b12-7+
InchiKey: UYBGOPSMJQAVEH-KPKJPENVSA-N
Formula: C12H13N
SMILES: CCCC=C(C#N)c1ccccc1
Mol. weight [g/mol]: 171.24
CAS: 6519-09-1

Physical Properties

Property code	Value	Unit	Source
chs	-6759.84	kJ/mol	NIST Webbook
gf	367.42	kJ/mol	Joback Method
hf	217.83	kJ/mol	Joback Method
hfs	179.70	kJ/mol	NIST Webbook
hfus	21.28	kJ/mol	Joback Method
hvap	55.10	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.394		Crippen Method
mcvol	153.260	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
tb	606.76	K	Joback Method
tc	835.59	K	Joback Method
tf	297.37	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.20	J/mol×K	606.76	Joback Method
cpg	374.91	J/mol×K	644.90	Joback Method
cpg	387.66	J/mol×K	683.04	Joback Method
cpg	399.52	J/mol×K	721.18	Joback Method
cpg	410.56	J/mol×K	759.31	Joback Method

cpg	420.84	J/mol×K	797.45	Joback Method
cpg	430.44	J/mol×K	835.59	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=C6519091&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