2-Phenyl-hept-2-enenitrile

Inchi: InChI=1S/C13H15N/c1-2-3-5-10-13(11-14)12-8-6-4-7-9-12/h4,6-10H,2-3,5H2,1H3/b13-1
InchiKey: YFEFSOGDFAEYCS-JLHYYAGUSA-N
Formula: C13H15N
SMILES: CCCCC=C(C#N)c1ccccc1
Mol. weight [g/mol]: 185.26
CAS: 6702-34-7

Physical Properties

Property code	Value	Unit	Source
chs	-7418.57	kJ/mol	NIST Webbook
gf	375.84	kJ/mol	Joback Method
hf	197.19	kJ/mol	Joback Method
hfs	159.10	kJ/mol	NIST Webbook
hfus	23.86	kJ/mol	Joback Method
hvap	57.32	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.784		Crippen Method
mcvol	167.350	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
tb	629.64	K	Joback Method
tc	854.13	K	Joback Method
tf	308.64	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.85	J/mol×K	629.64	Joback Method
cpg	424.21	J/mol×K	667.06	Joback Method
cpg	437.61	J/mol×K	704.47	Joback Method
cpg	450.10	J/mol×K	741.89	Joback Method
cpg	461.76	J/mol×K	779.30	Joback Method
cpg	472.65	J/mol×K	816.72	Joback Method
cpg	482.84	J/mol×K	854.13	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=C6702347&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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