6-Phenylhexanenitrile

Inchi: InChI=1S/C12H15N/c13-11-7-2-1-4-8-12-9-5-3-6-10-12/h3,5-6,9-10H,1-2,4,7-8H2
InchiKey: BSJKBXNHLQEFMG-UHFFFAOYSA-N
Formula: C12H15N
SMILES: N#CCCCCCc1ccccc1
Mol. weight [g/mol]: 173.25
CAS: 17777-31-0

Physical Properties

Property code	Value	Unit	Source
gf	295.75	kJ/mol	Joback Method
hf	110.40	kJ/mol	Joback Method
hfus	22.38	kJ/mol	Joback Method
hvap	55.06	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.313		Crippen Method
mcvol	157.560	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	1568.10		NIST Webbook
tb	602.72	K	Joback Method
tc	818.18	K	Joback Method
tf	316.41	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.06	J/mol×K	602.72	Joback Method
cpg	396.17	J/mol×K	638.63	Joback Method
cpg	409.41	J/mol×K	674.54	Joback Method
cpg	421.81	J/mol×K	710.45	Joback Method
cpg	433.41	J/mol×K	746.36	Joback Method
cpg	444.26	J/mol×K	782.27	Joback Method
cpg	454.40	J/mol×K	818.18	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=C17777310&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume