4-Phenylpiperidine

Other names: Piperidine, 4-phenyl-
Inchi: InChI=1S/C11H15N/c1-2-4-10(5-3-1)11-6-8-12-9-7-11/h1-5,11-12H,6-9H2
InchiKey: UTBULQCHEUWJNV-UHFFFAOYSA-N
Formula: C11H15N
SMILES: c1ccc(C2CCNCC2)cc1
Mol. weight [g/mol]: 161.24
CAS: 771-99-3

Physical Properties

Property code	Value	Unit	Source
gf	266.31	kJ/mol	Joback Method
hf	58.29	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	49.54	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.154		Crippen Method
mcvol	141.210	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
rinpol	1454.00		NIST Webbook
rinpol	1454.00		NIST Webbook
tb	545.86	K	Joback Method
tc	795.99	K	Joback Method
tf	352.56	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.31	J/mol×K	545.86	Joback Method
cpg	352.58	J/mol×K	587.55	Joback Method
cpg	371.43	J/mol×K	629.24	Joback Method
cpg	388.90	J/mol×K	670.93	Joback Method
cpg	405.04	J/mol×K	712.61	Joback Method
cpg	419.92	J/mol×K	754.30	Joback Method

cpg	433.57	J/mol×K	795.99	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	529.20	K	96.90	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C771993&Units=SI

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume