Pyrimidine, 4-phenyl-

Other names: 4-Phenylpyrimidine
Inchi: InChI=1S/C10H8N2/c1-2-4-9(5-3-1)10-6-7-11-8-12-10/h1-8H
InchiKey: MKLQPIYLZMLAER-UHFFFAOYSA-N
Formula: C10H8N2
SMILES: c1ccc(-c2ccncn2)cc1
Mol. weight [g/mol]: 156.18
CAS: 3438-48-0

Physical Properties

Property code	Value	Unit	Source
hfus	18.80	kJ/mol	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds
hvap	68.80 ± 2.50	kJ/mol	NIST Webbook
ie	8.65	eV	NIST Webbook
ie	9.42	eV	NIST Webbook
log10ws	-3.61		Crippen Method
logp	2.144		Crippen Method
mcvol	124.200	ml/mol	McGowan Method
rinpol	1432.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	18.80	kJ/mol	334.10	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3438480&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds:	https://www.doi.org/10.1021/je900034d

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices