4-PHENETHYLPYRIDINE

Other names: 4-(2-Phenylethyl)pyridine
Inchi: InChI=1S/C13H13N/c1-2-4-12(5-3-1)6-7-13-8-10-14-11-9-13/h1-5,8-11H,6-7H2
InchiKey: UWLBLNRDXXHYGS-UHFFFAOYSA-N
Formula: C13H13N
SMILES: c1ccc(CCc2ccncc2)cc1
Mol. weight [g/mol]: 183.25

Physical Properties

Property code	Value	Unit	Source
af	0.4677		Cheméo Relay (1.0)
gf	311.32	kJ/mol	Cheméo Relay (1.0, beta)
hf	215.86	kJ/mol	Cheméo Relay (1.0)
hvap	81.94	kJ/mol	Cheméo Relay (1.0)
ie	9.17	eV	Cheméo Relay (1.0)
log10ws	-2.36		Cheméo Relay (1.0)
logp	2.867		Crippen Method
mcvol	156.490	ml/mol	McGowan Method
pc	3168.04	kPa	Cheméo Relay (1.0, beta)
rinpol	1603.00		NIST Webbook
tb	568.98	K	Cheméo Relay (1.0)
tc	819.90	K	Cheméo Relay (1.0)
tf	304.96	K	Cheméo Relay (1.0)
vc	0.594	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2116645&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume