4-Piperidinecarboxylic acid, 4-phenyl-, ethyl ester

Other names: Isonipecotic acid, 4-phenyl-, ethyl ester
Ethyl 4-phenylisonipecotate
Ethyl 4-phenylpiperidine-4-carboxylate
Nordolsin
Normeperidine
Norpethidine
4-(Ethoxycarbonyl)-4-phenylpiperidine
4-Carbethoxy-4-phenylpiperidine
4-Phenyl-4-carbethoxypiperidine
Ethyl 4-phenyl-4-piperidinecarboxylate

Inchi: InChI=1S/C14H19NO2/c1-2-17-13(16)14(8-10-15-11-9-14)12-6-4-3-5-7-12/h3-7,15H,2,8-

InchiKey: QKHMFBKXTNQCTM-UHFFFAOYSA-N

Formula: C14H19NO2

SMILES: CCOC(=O)C1(c2ccccc2)CCNCC1

Mol. weight [g/mol]: 233.31

CAS: 77-17-8

Physical Properties

Property code	Value	Unit	Source
gf	52.16	kJ/mol	Joback Method
hf	-233.19	kJ/mol	Joback Method
hfus	23.97	kJ/mol	Joback Method
hvap	64.23	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.871		Crippen Method
mcvol	190.920	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	1745.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1738.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1738.00		NIST Webbook
rinpol	1738.00		NIST Webbook
rinpol	1738.00		NIST Webbook
rinpol	1749.00		NIST Webbook

tb	691.03	K	Joback Method
tc	937.41	K	Joback Method
tf	482.43	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.36	J/mol×K	691.03	Joback Method
cpg	550.36	J/mol×K	732.09	Joback Method
cpg	568.24	J/mol×K	773.16	Joback Method
cpg	585.17	J/mol×K	814.22	Joback Method
cpg	601.30	J/mol×K	855.28	Joback Method
cpg	616.80	J/mol×K	896.35	Joback Method
cpg	631.84	J/mol×K	937.41	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77178&Units=SI
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

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