N-PHENETHYLFORMAMIDE

Other names:	N-Formylphenylethylamine
	Formamide, N-phenethyl-,
	2-Phenylethylformamide
	(2-Phenethyl)formamide
	N-(2-Phenethyl)formamide
	N-(2'-phenylethyl)formamide
	Phenylethyl formamide
Inchi:	InChI=1S/C9H11NO/c11-8-10-7-6-9-4-2-1-3-5-9/h1-5,8H,6-7H2,(H,10,11)
InchiKey:	NOOOMJZHMKSKBF-UHFFFAOYSA-N
Formula:	C9H11NO
SMILES:	O=CNCCc1ccccc1
Mol. weight [g/mol]:	149.19

Physical Properties

Property code	Value	Unit	Source
af	0.5101		Cheméo Relay (1.0)
gf	127.18	kJ/mol	Joback Method
hf	-72.14	kJ/mol	Cheméo Relay (1.0)
hfus	20.50	kJ/mol	Joback Method
hvap	76.38	kJ/mol	Cheméo Relay (1.0)
ie	9.22	eV	Cheméo Relay (1.0)
log10ws	-1.09		Cheméo Relay (1.0)
logp	0.975		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	1487.20		NIST Webbook
tb	555.42	K	Cheméo Relay (1.0)
tc	781.71	K	Cheméo Relay (1.0)
tf	282.81	K	Cheméo Relay (1.0)
vc	0.450	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	279.55	J/mol×K	530.83	Joback Method
cpg	292.25	J/mol×K	566.42	Joback Method
cpg	304.14	J/mol×K	602.01	Joback Method
cpg	315.27	J/mol×K	637.60	Joback Method
cpg	325.66	J/mol×K	673.19	Joback Method
cpg	335.35	J/mol×K	708.78	Joback Method
cpg	344.37	J/mol×K	744.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23069990&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
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
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