FORMAMIDE, N-(1-PHENYLETHYL)-

Other names: Formamide, N-(1-phenylethyl)-
N-Phenylethylformamide
N-(1-phenylethyl)formamide
Inchi: InChI=1S/C9H11NO/c1-8(10-7-11)9-5-3-2-4-6-9/h2-8H,1H3,(H,10,11)
InchiKey: CDHCCWRMWKZBGE-UHFFFAOYSA-N
Formula: C9H11NO
SMILES: CC(NC=O)c1ccccc1
Mol. weight [g/mol]: 149.19

Physical Properties

Property code	Value	Unit	Source
af	0.4324		Cheméo Relay (1.0)
gf	124.74	kJ/mol	Joback Method
hf	-108.99	kJ/mol	Cheméo Relay (1.0)
hfus	16.97	kJ/mol	Joback Method
hvap	77.28	kJ/mol	Cheméo Relay (1.0)
ie	8.99	eV	Cheméo Relay (1.0)
log10ws	-1.63		Cheméo Relay (1.0)
logp	1.494		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
tb	525.31	K	Cheméo Relay (1.0)
tc	757.59	K	Cheméo Relay (1.0)
tf	296.53	K	Cheméo Relay (1.0)
vc	0.440	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.87	J/mol×K	530.39	Joback Method
cpg	292.93	J/mol×K	566.78	Joback Method
cpg	305.14	J/mol×K	603.18	Joback Method
cpg	316.53	J/mol×K	639.57	Joback Method
cpg	327.14	J/mol×K	675.96	Joback Method

cpg	337.01	J/mol×K	712.36	Joback Method
cpg	346.18	J/mol×K	748.75	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6948012&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume