PROPANAMIDE, N-PHENYL-

Other names:	N-Phenylpropionamide
	Propionamide, N-phenyl-
	Propionanilide
Inchi:	InChI=1S/C9H11NO/c1-2-9(11)10-8-6-4-3-5-7-8/h3-7H,2H2,1H3,(H,10,11)
InchiKey:	ZTHRQJQJODGZHV-UHFFFAOYSA-N
Formula:	C9H11NO
SMILES:	CCC(=O)Nc1ccccc1
Mol. weight [g/mol]:	149.19

Physical Properties

Property code	Value	Unit	Source
hf	-144.79	kJ/mol	Cheméo Relay (1.0)
hfus	19.81	kJ/mol	Joback Method
hvap	62.95	kJ/mol	Cheméo Relay (1.0)
ie	8.30	eV	Cheméo Relay (1.0)
log10ws	-1.92		Aqueous Solubility Prediction Method
logp	2.035		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
tb	525.22	K	Cheméo Relay (1.0)
tc	766.71	K	Cheméo Relay (1.0)
tf	378.65	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.38	J/mol×K	536.04	Joback Method
cpg	291.41	J/mol×K	572.52	Joback Method
cpg	303.61	J/mol×K	609.00	Joback Method
cpg	315.00	J/mol×K	645.47	Joback Method
cpg	325.61	J/mol×K	681.95	Joback Method
cpg	335.50	J/mol×K	718.43	Joback Method
cpg	344.69	J/mol×K	754.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C620713&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point