N-(«alpha»-Methylbenzyl)-formamide

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
CAS:	6948-01-2

Physical Properties

Property code	Value	Unit	Source
gf	124.74	kJ/mol	Joback Method
hf	-29.95	kJ/mol	Joback Method
hfus	16.97	kJ/mol	Joback Method
hvap	50.67	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.494		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
tb	530.39	K	Joback Method
tc	748.75	K	Joback Method
tf	297.27	K	Joback Method
vc	0.477	m3/kmol	Joback Method

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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6948012&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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