N-(4-methoxybenzyl)formamide

Inchi: InChI=1S/C9H11NO2/c1-12-9-4-2-8(3-5-9)6-10-7-11/h2-5,7H,6H2,1H3,(H,10,11)
InchiKey: DATDKKQVOOSHGC-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: COc1ccc(CN=CO)cc1
Mol. weight [g/mol]: 165.19
CAS: 17061-63-1

Physical Properties

Property code	Value	Unit	Source
hf	-206.26	kJ/mol	Joback Method
hvap	60.97	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.781		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1674.10		NIST Webbook
rinpol	1674.10		NIST Webbook
tb	628.26	K	Joback Method
tc	837.87	K	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=C17061631&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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