N-(3-Methoxybenzyl)acetamide

Inchi: InChI=1S/C10H13NO2/c1-8(12)11-7-9-4-3-5-10(6-9)13-2/h3-6H,7H2,1-2H3,(H,11,12)
InchiKey: QISBKEXGALSAAL-UHFFFAOYSA-N
Formula: C10H13NO2
SMILES: COc1cccc(CN=C(C)O)c1
Mol. weight [g/mol]: 179.22
CAS: 174688-81-4

Physical Properties

Property code	Value	Unit	Source
hf	-236.69	kJ/mol	Joback Method
hvap	63.28	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.172		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1686.50		NIST Webbook
rinpol	1686.50		NIST Webbook
tb	651.02	K	Joback Method
tc	860.75	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C174688814&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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