

Acetamide, N-(4-methoxyphenyl)-2-methoxy-

Inchi:	InChI=1S/C10H13NO3/c1-13-7-10(12)11-8-3-5-9(14-2)6-4-8/h3-6H,7H2,1-2H3,(H,11,12)
InchiKey:	TTZFXJGNEYPIBY-UHFFFAOYSA-N
Formula:	C10H13NO3
SMILES:	COCC(=O)Nc1ccc(OC)cc1
Mol. weight [g/mol]:	195.22

Physical Properties

Property code	Value	Unit	Source
gf	-113.43	kJ/mol	Joback Method
hf	-348.22	kJ/mol	Joback Method
hfus	24.38	kJ/mol	Joback Method
hvap	58.79	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	1.280		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	1719.00		NIST Webbook
rinpol	1719.00		NIST Webbook
tb	608.74	K	Joback Method
tc	820.04	K	Joback Method
tf	388.45	K	Joback Method
vc	0.565	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.89	J/mol×K	608.74	Joback Method
cpg	384.97	J/mol×K	643.96	Joback Method
cpg	397.32	J/mol×K	679.17	Joback Method
cpg	408.96	J/mol×K	714.39	Joback Method
cpg	419.87	J/mol×K	749.61	Joback Method
cpg	430.05	J/mol×K	784.82	Joback Method
cpg	439.52	J/mol×K	820.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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