

methyl (4-nitrophenyl)carbamate

Inchi:	InChI=1S/C8H8N2O4/c1-14-8(11)9-6-2-4-7(5-3-6)10(12)13/h2-5H,1H3,(H,9,11)
InchiKey:	DAWCBJXIGOELKF-UHFFFAOYSA-N
Formula:	C8H8N2O4
SMILES:	COC(=O)Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	196.16
CAS:	1943-87-9

Physical Properties

Property code	Value	Unit	Source
chs	-3863.50 ± 4.60	kJ/mol	NIST Webbook
gf	10.28	kJ/mol	Joback Method
hf	-185.48	kJ/mol	Joback Method
hfs	-427.90 ± 4.60	kJ/mol	NIST Webbook
hfus	29.38	kJ/mol	Joback Method
hvap	68.52	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	1.773		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
tb	692.40	K	Joback Method
tc	936.99	K	Joback Method
tf	487.29	K	Joback Method
vc	0.516	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.80	J/mol×K	692.40	Joback Method
cpg	353.23	J/mol×K	733.16	Joback Method
cpg	362.81	J/mol×K	773.93	Joback Method
cpg	371.54	J/mol×K	814.69	Joback Method
cpg	379.44	J/mol×K	855.46	Joback Method
cpg	386.54	J/mol×K	896.22	Joback Method
cpg	392.86	J/mol×K	936.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1943879&Units=SI&Mask=3FFF
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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

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