P-methoxy carbanilic acid, ethyl ester

Other names: Carbamic acid, 4-methoxyphenyl, ethyl ester
Inchi: InChI=1S/C10H13NO3/c1-3-14-10(12)11-8-4-6-9(13-2)7-5-8/h4-7H,3H2,1-2H3,(H,11,12)
InchiKey: KUGFZNSGTFZXML-UHFFFAOYSA-N
Formula: C10H13NO3
SMILES: CCOC(=O)Nc1ccc(OC)cc1
Mol. weight [g/mol]: 195.22
CAS: 7451-55-0

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	-2.28		Crippen Method
logp	2.264		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	1632.00		NIST Webbook
rinpol	1639.00		NIST Webbook
rinpol	1636.00		NIST Webbook
tb	608.74	K	Joback Method
tc	820.04	K	Joback Method
tf	388.45	K	Joback Method
vc	0.565	m3/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=C7451550&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

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