N,N,2,6-Tetramethylaniline,4-carboxylic acid, methyl ester

Inchi: InChI=1S/C12H17NO2/c1-8-6-10(12(14)15-5)7-9(2)11(8)13(3)4/h6-7H,1-5H3
InchiKey: WIJWZUPWOWXGTD-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: COC(=O)c1cc(C)c(N(C)C)c(C)c1
Mol. weight [g/mol]: 207.27
CAS: 56066-86-5

Physical Properties

Property code	Value	Unit	Source
affp	945.40	kJ/mol	NIST Webbook
basg	913.00	kJ/mol	NIST Webbook
gf	10.54	kJ/mol	Joback Method
hf	-266.16	kJ/mol	Joback Method
hfus	25.52	kJ/mol	Joback Method
hvap	57.77	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.156		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
tb	604.31	K	Joback Method
tc	810.42	K	Joback Method
tf	393.61	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.56	J/mol×K	604.31	Joback Method
cpg	444.50	J/mol×K	638.66	Joback Method
cpg	458.64	J/mol×K	673.01	Joback Method
cpg	472.00	J/mol×K	707.36	Joback Method
cpg	484.61	J/mol×K	741.72	Joback Method
cpg	496.46	J/mol×K	776.07	Joback Method
cpg	507.58	J/mol×K	810.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56066865&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

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume