Benzoic acid, 4-(dimethylamino)-, methyl ester

Other names:	4-(CH3)2NC6H4COOCH3
	4-(dimethylamino)benzoic acid, methyl ester
	Benzoic acid, p-(dimethylamino)-, methyl ester
	Methyl 4-(N,N-dimethylamino)benzoate
	Methyl 4-(dimethylamino)benzoate
	Methyl p-(dimethylamino)benzoate
Inchi:	InChI=1S/C10H13NO2/c1-11(2)9-6-4-8(5-7-9)10(12)13-3/h4-7H,1-3H3
InchiKey:	DBQGARDMYOMOOS-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	COC(=O)c1ccc(N(C)C)cc1
Mol. weight [g/mol]:	179.22
CAS:	1202-25-1

Physical Properties

Property code	Value	Unit	Source
affp	920.60	kJ/mol	NIST Webbook
basg	894.10	kJ/mol	NIST Webbook
gf	12.96	kJ/mol	Joback Method
hf	-201.94	kJ/mol	Joback Method
hfus	23.40	kJ/mol	Vapor Pressures and Phase Diagrams of Two Methyl Esters of Substituted Benzoic Acids
hvap	51.99	kJ/mol	Joback Method
log10ws	-2.38		Aqueous Solubility Prediction Method
logp	1.539		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
tb	548.59	K	Joback Method
tc	759.30	K	Joback Method
tf	371.70 ± 0.50	K	NIST Webbook
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.56	J/mol×K	548.59	Joback Method
cpg	348.54	J/mol×K	583.71	Joback Method
cpg	361.71	J/mol×K	618.83	Joback Method
cpg	374.11	J/mol×K	653.94	Joback Method
cpg	385.75	J/mol×K	689.06	Joback Method
cpg	396.66	J/mol×K	724.18	Joback Method
cpg	406.85	J/mol×K	759.30	Joback Method
hfust	26.07	kJ/mol	371.80	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1202251&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor Pressures and Phase Diagrams of Two Methyl Esters of Substituted Benzoic Acids:	https://www.doi.org/10.1021/je2007605
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion at a given temperature
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