Benzoic acid, 3-(dimethylamino)-, methyl ester

Inchi: InChI=1S/C10H13NO2/c1-11(2)9-6-4-5-8(7-9)10(12)13-3/h4-7H,1-3H3
InchiKey: CABFTHPIDKWPNQ-UHFFFAOYSA-N
Formula: C10H13NO2
SMILES: COC(=O)c1cccc(N(C)C)c1
Mol. weight [g/mol]: 179.22

Physical Properties

Property code	Value	Unit	Source
gf	12.96	kJ/mol	Joback Method
hf	-201.94	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	51.99	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.539		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1559.00		NIST Webbook
rinpol	1559.00		NIST Webbook
tb	548.59	K	Joback Method
tc	759.30	K	Joback Method
tf	346.03	K	Joback Method
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

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374477&Units=SI

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