Benzoic acid, 2-(formylamino)-, methyl ester

Other names:	Methyl N-formylanthranilate
	Methyl 2-formylaminobenzoate
	Methyl 2-formamidobenzoate
Inchi:	InChI=1S/C9H9NO3/c1-13-9(12)7-4-2-3-5-8(7)10-6-11/h2-6H,1H3,(H,10,11)
InchiKey:	HRNPZFOYXWWMFL-UHFFFAOYSA-N
Formula:	C9H9NO3
SMILES:	COC(=O)c1ccccc1NC=O
Mol. weight [g/mol]:	179.17
CAS:	41270-80-8

Physical Properties

Property code	Value	Unit	Source
gf	-116.37	kJ/mol	Joback Method
hf	-280.94	kJ/mol	Joback Method
hfus	22.89	kJ/mol	Joback Method
hvap	60.88	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.041		Crippen Method
mcvol	132.900	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
rinpol	1564.10		NIST Webbook
rinpol	1564.10		NIST Webbook
tb	612.10	K	Joback Method
tc	832.00	K	Joback Method
tf	396.95	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.66	J/mol×K	612.10	Joback Method
cpg	326.58	J/mol×K	648.75	Joback Method
cpg	336.79	J/mol×K	685.40	Joback Method
cpg	346.31	J/mol×K	722.05	Joback Method

cpg	355.15	J/mol×K	758.70	Joback Method
cpg	363.33	J/mol×K	795.35	Joback Method
cpg	370.85	J/mol×K	832.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41270808&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