5-Methoxyanthranilic acid

Other names: 2-Amino-5-methoxybenzoic acid
Inchi: InChI=1S/C8H9NO3/c1-12-5-2-3-7(9)6(4-5)8(10)11/h2-4H,9H2,1H3,(H,10,11)
InchiKey: UMKSAURFQFUULT-UHFFFAOYSA-N
Formula: C8H8NO3
SMILES: COc1ccc(N)c(C(=O)O)c1
Mol. weight [g/mol]: 166.15
CAS: 6705-03-9

Physical Properties

Property code	Value	Unit	Source
gf	-194.66	kJ/mol	Joback Method
hf	-358.10	kJ/mol	Joback Method
hfus	22.88	kJ/mol	Thermodynamic Study on the Sublimation of Five Aminomethoxybenzoic Acids
hsub	119.30 ± 0.80	kJ/mol	NIST Webbook
hvap	73.48	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	0.976		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
tb	660.08	K	Joback Method
tc	873.76	K	Joback Method
tf	447.62	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.56	J/mol×K	838.14	Joback Method
cpg	306.33	J/mol×K	660.08	Joback Method
cpg	315.27	J/mol×K	695.69	Joback Method
cpg	323.66	J/mol×K	731.31	Joback Method
cpg	331.50	J/mol×K	766.92	Joback Method

cpg	338.80	J/mol×K	802.53	Joback Method
cpg	351.78	J/mol×K	873.76	Joback Method
hfust	22.88	kJ/mol	425.00	NIST Webbook
hsubt	116.90 ± 0.80	kJ/mol	364.00	NIST Webbook

Sources

Thermodynamic Study on the Sublimation of Five Aminomethoxybenzoic Acids:	https://www.doi.org/10.1021/je9004036
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=C6705039&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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

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