2-Amino-5-methylbenzoic acid

Other names:	5-Methylanthranilic acid
	Benzoic acid, 2-amino-5-methyl-
	m-Toluic acid, 6-amino-
	6-amino-m-toluic acid
Inchi:	InChI=1S/C8H9NO2/c1-5-2-3-7(9)6(4-5)8(10)11/h2-4H,9H2,1H3,(H,10,11)
InchiKey:	NBUUUJWWOARGNW-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	Cc1ccc(N)c(C(=O)O)c1
Mol. weight [g/mol]:	151.16
CAS:	2941-78-8

Physical Properties

Property code	Value	Unit	Source
gf	-89.66	kJ/mol	Joback Method
hf	-225.88	kJ/mol	Joback Method
hfus	20.62	kJ/mol	Joback Method
hsub	110.60 ± 1.90	kJ/mol	NIST Webbook
hvap	71.07	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.275		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
tb	637.66	K	Joback Method
tc	853.80	K	Joback Method
tf	425.39	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.29	J/mol×K	637.66	Joback Method
cpg	293.26	J/mol×K	673.68	Joback Method
cpg	301.67	J/mol×K	709.71	Joback Method
cpg	309.53	J/mol×K	745.73	Joback Method

cpg	316.86	J/mol×K	781.76	Joback Method
cpg	323.68	J/mol×K	817.78	Joback Method
cpg	330.01	J/mol×K	853.80	Joback Method
hfust	27.63	kJ/mol	450.00	NIST Webbook
hsubt	108.90 ± 0.50	kJ/mol	353.00	NIST Webbook

Sources

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=C2941788&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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