Atropic acid

Other names:	2-Phenylacrylic acid
	2-Propenoic acid, 2-phenyl-
	Acrylic acid, 2-phenyl-
	Benzeneacetic acid, «alpha»-methylene-
	Benzeneacetic acid, Â«alphaÂ»-methylene-
	NSC 20987
	Propenoic acid, 2-phenyl-
	«alpha»-Phenylacrylic acid
	«alpha»-Toluic acid, «alpha»-methylene-
	Â«alphaÂ»-Phenylacrylic acid
	Â«alphaÂ»-Toluic acid, Â«alphaÂ»-methylene-
Inchi:	InChI=1S/C9H8O2/c1-7(9(10)11)8-5-3-2-4-6-8/h2-6H,1H2,(H,10,11)
InchiKey:	ONPJWQSDZCGSQM-UHFFFAOYSA-N
Formula:	C9H8O2
SMILES:	C=C(C(=O)O)c1ccccc1
Mol. weight [g/mol]:	148.16
CAS:	492-38-6

Physical Properties

Property code	Value	Unit	Source
gf	-49.14	kJ/mol	Joback Method
hf	-141.73	kJ/mol	Joback Method
hfus	16.20	kJ/mol	Joback Method
hvap	60.74	kJ/mol	Joback Method
log10ws	-2.06		Aqueous Solubility Prediction Method
logp	1.784		Crippen Method
mcvol	117.050	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
tb	574.61	K	Joback Method
tc	785.54	K	Joback Method
tf	379.65	K	Aqueous Solubility Prediction Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.34	J/mol×K	574.61	Joback Method
cpg	271.27	J/mol×K	609.77	Joback Method
cpg	280.51	J/mol×K	644.92	Joback Method
cpg	289.10	J/mol×K	680.08	Joback Method
cpg	297.10	J/mol×K	715.23	Joback Method
cpg	304.52	J/mol×K	750.39	Joback Method
cpg	311.40	J/mol×K	785.54	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
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=C492386&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume