Risocaine

Other names:	4-(Propoxycarbonyl)aniline
	Benzoic acid, 4-amino-, propyl ester
	Benzoic acid, p-amino-, propyl ester
	Keloform P
	NSC-23516
	Propaesin
	Propazyl
	Propesin
	Propesine
	Propyl 4-aminobenzoate
	Propyl-p-amino benzoate
	Propylcain
	Raythesin
	n-Propyl p-aminobenzoate
	n-Propyl-4-aminobenzoate
	p-Aminobenzoic acid, propyl ester
	propyl-p-aminobenzoate
Inchi:	InChI=1S/C10H13NO2/c1-2-7-13-10(12)8-3-5-9(11)6-4-8/h3-6H,2,7,11H2,1H3
InchiKey:	NBFQYHKHPBMJJV-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CCCOC(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	179.22
CAS:	94-12-2

Physical Properties

Property code	Value	Unit	Source
gf	-31.37	kJ/mol	Joback Method
hf	-235.68	kJ/mol	Joback Method
hfus	23.29	kJ/mol	Joback Method
hvap	60.59	kJ/mol	Joback Method
log10ws	-2.45		Estimated Solubility Method
log10ws	-2.33		Aqueous Solubility Prediction Method
logp	1.836		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method

rinpol	1659.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1670.00		NIST Webbook
tb	608.68	K	Joback Method
tc	830.79	K	Joback Method
tf	347.65	K	Aqueous Solubility Prediction Method
tf	346.00 ± 1.00	K	NIST Webbook
tf	347.00 ± 0.50	K	NIST Webbook
tf	345.80 ± 0.50	K	NIST Webbook
tf	346.00 ± 0.50	K	NIST Webbook
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.09	J/mol×K	608.68	Joback Method
cpg	370.13	J/mol×K	645.70	Joback Method
cpg	382.38	J/mol×K	682.72	Joback Method
cpg	393.85	J/mol×K	719.74	Joback Method
cpg	404.56	J/mol×K	756.76	Joback Method
cpg	414.52	J/mol×K	793.78	Joback Method
cpg	423.76	J/mol×K	830.79	Joback Method
hfust	20.54	kJ/mol	347.10	NIST Webbook
hfust	20.54	kJ/mol	347.10	NIST Webbook
sfust	64.61	J/mol×K	347.10	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C94122&Units=SI

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

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
hfust:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume