Probenecid

Other names:	4-((Dipropylamino)sulfonyl)benzoic acid
	4-(Dipropylsulfamoyl)benzoic acid
	4-(N,N-dipropylaminosulfonyl)benzoic acid
	4-(N,N-dipropylsulfamoyl)benzoic acid
	4-[(Dipropylamino)sulfonyl]benzoic acid (probenecid)
	Apurina
	Benecid
	Benemid
	Benuryl
	Benzoic acid, 4-[(dipropylamino)sulfonyl]-
	Benzoic acid, p-(dipropylsulfamoyl)-
	Ethamide
	NCI-C56097
	NSC 18786
	Probecid
	Proben
	Probenecid acid
	Probenemid
	Probexin
	Prolongine
	Synergid R
	Tubophan
	Uricosid
	p-(Dipropylsulfamoyl)benzoic acid
	p-(Dipropylsulfamyl)benzoic acid
Inchi:	InChI=1S/C13H19NO4S/c1-3-9-14(10-4-2)19(17,18)12-7-5-11(6-8-12)13(15)16/h5-8H,3-
InchiKey:	DBABZHXKTCFAPX-UHFFFAOYSA-N
Formula:	C13H19NO4S
SMILES:	CCCN(CCC)S(=O)(=O)c1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	285.36
CAS:	57-66-9

Physical Properties

Property code	Value	Unit	Source
gf	-462.14	kJ/mol	Joback Method
hf	-737.22	kJ/mol	Joback Method

hfus	43.16	kJ/mol	Joback Method
hvap	91.57	kJ/mol	Joback Method
log10ws	-4.02		Aqueous Solubility Prediction Method
log10ws	-4.86		Aqueous Solubility Prediction Method
logp	2.195		Crippen Method
mcvol	215.780	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
rinpol	2336.00		NIST Webbook
rinpol	2336.00		NIST Webbook
tb	734.77	K	Joback Method
tc	924.28	K	Joback Method
tf	469.90	K	Aqueous Solubility Prediction Method
tf	469.90	K	Aqueous Solubility Prediction Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.29	J/mol×K	734.77	Joback Method
cpg	614.08	J/mol×K	766.36	Joback Method
cpg	626.01	J/mol×K	797.94	Joback Method
cpg	637.10	J/mol×K	829.53	Joback Method
cpg	647.37	J/mol×K	861.11	Joback Method
cpg	656.85	J/mol×K	892.70	Joback Method
cpg	665.55	J/mol×K	924.28	Joback Method
hfust	33.57	kJ/mol	471.00	NIST Webbook
hfust	40.90	kJ/mol	472.10	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility Measurement and Correlation of Probenecid in 12 Pure Organic Solvents and Thermodynamic Properties of Mixing of Solutions:	https://www.doi.org/10.1021/acs.jced.8b00863
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume