Thiambutosine

Other names:	Thiourea, N-(4-butoxyphenyl)-N'-[4-(dimethylamino)phenyl]-
	Carbanilide, 4-butoxy-4'-(dimethylamino)thio-
	Ciba 1906
	Su 1906
	Summit 1906
	Thiambutosin
	4-Butoxy-4'-(dimethylamino)thiocarbanilide
	1-(p-Butoxyphenyl)-3-(p-dimethylaminophenyl)-2-thiourea
	1-(4-Butoxyphenyl)-3-(4-dimethylaminophenyl)thiourea
	Thaimbutosine
	NSC 682
Inchi:	InChI=1S/C19H25N3OS/c1-4-5-14-23-18-12-8-16(9-13-18)21-19(24)20-15-6-10-17(11-7-
InchiKey:	JYCBKPOKWDDOOV-UHFFFAOYSA-N
Formula:	C19H25N3OS
SMILES:	CCCCOc1ccc(NC(=S)Nc2ccc(N(C)C)cc2)cc1
Mol. weight [g/mol]:	343.49
CAS:	500-89-0

Physical Properties

Property code	Value	Unit	Source
gf	616.28	kJ/mol	Joback Method
hf	203.38	kJ/mol	Joback Method
hfus	51.28	kJ/mol	Joback Method
hvap	87.82	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.740		Crippen Method
mcvol	278.910	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
tb	902.68	K	Joback Method
tc	1134.08	K	Joback Method
tf	576.06	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.22	J/mol×K	902.68	Joback Method
cpg	860.98	J/mol×K	941.25	Joback Method
cpg	874.77	J/mol×K	979.81	Joback Method
cpg	887.69	J/mol×K	1018.38	Joback Method
cpg	899.87	J/mol×K	1056.95	Joback Method
cpg	911.41	J/mol×K	1095.52	Joback Method
cpg	922.42	J/mol×K	1134.08	Joback Method

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=C500890&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
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