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]:	343.50

Physical Properties

Property code	Value	Unit	Source
hfus	51.28	kJ/mol	Joback Method
ie	6.39	eV	Cheméo Relay (1.0)
logp	4.740		Crippen Method
mcvol	278.910	ml/mol	McGowan Method
tb	692.52	K	Cheméo Relay (1.0)
tf	443.67	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C500890&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point