Tribromsalan

Other names:	3,5,4'-Tribromosalicylanilide
	3,4',5-Tribromosalicylanilide
	Benzamide, 3,5-dibromo-N-(4-bromophenyl)-2-hydroxy-
	Agramed
	ET-394
	Salicylanilide, 3,4',5-tribromo-
	Sherstat TBS
	Temasept II
	Temasept IV
	Tempasept II
	Tribromosalicylanilide
	Tribromsalen
	Trisanil
	Trisanyl
	Tuasal 100
	Tuasol
	Tuasol 100
	TBS
	TBS 95
	Vancide TBS
	3,4',5-Tribromosalicylanide
	3,5-Dibromosalicylic acid p-bromoanilide
	3,5-Dibromo-N-(4-bromophenyl)-2-hydroxybenzamide
	ASC-4
	Lamar L-300
	Tuasal
	WR 34912
	NSC 20526
Inchi:	InChI=1S/C13H8Br3NO2/c14-7-1-3-9(4-2-7)17-13(19)10-5-8(15)6-11(16)12(10)18/h1-6,1
InchiKey:	KVSKGMLNBAPGKH-UHFFFAOYSA-N
Formula:	C13H8Br3NO2
SMILES:	O=C(Nc1ccc(Br)cc1)c1cc(Br)cc(Br)c1O
Mol. weight [g/mol]:	449.92
CAS:	87-10-5

Physical Properties

Property code	Value	Unit	Source

gf	103.32	kJ/mol	Joback Method
hf	-30.43	kJ/mol	Joback Method
hfus	44.68	kJ/mol	Joback Method
hvap	96.57	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	4.932		Crippen Method
mcvol	216.430	ml/mol	McGowan Method
pc	4980.35	kPa	Joback Method
tb	948.28	K	Joback Method
tc	1231.36	K	Joback Method
tf	499.58 ± 0.20	K	NIST Webbook
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.07	J/mol×K	948.28	Joback Method
cpg	518.47	J/mol×K	995.46	Joback Method
cpg	527.96	J/mol×K	1042.64	Joback Method
cpg	537.77	J/mol×K	1089.82	Joback Method
cpg	548.11	J/mol×K	1137.00	Joback Method
cpg	559.21	J/mol×K	1184.18	Joback Method
cpg	571.31	J/mol×K	1231.36	Joback Method
hfust	28.67	kJ/mol	497.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C87105&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume