3,4',5-TRIBROMOSALICYLANILIDE

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

Physical Properties

Property code	Value	Unit	Source

hf	-123.79	kJ/mol	Cheméo Relay (1.0)
hfus	44.68	kJ/mol	Joback Method
ie	7.73	eV	Cheméo Relay (1.0)
log10ws	-5.87		Cheméo Relay (1.0)
logp	4.932		Crippen Method
mcvol	216.430	ml/mol	McGowan Method
tf	474.84	K	Cheméo Relay (1.0)

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

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C87105

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

cpg: Ideal gas heat capacity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

ie: Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point