

Triclocarban

Other names:	Urea, N-(4-chlorophenyl)-N'-(3,4-dichlorophenyl)- Carbanilide, 3,4,4'-trichloro- Cusiter Cutisan ENT 26925 Genoface Procutene TCC 3,4,4'-Trichlorocarbanilide 3,4,4'-Trichlorodiphenylurea 1-(4-Chlorophenyl)-3-(3,4-dichlorophenyl)urea CP 78416 N-(3,4-Dichlorophenyl)-N'-(4-chlorophenyl)urea Trilocarban NSC-72005 Solubacter 1-(3',4'-Dichlorophenyl)-3-(4'-chlorophenyl)urea N-(4-Chlorophenyl)-N'-(3,4-dichlorophenyl)urea Nipaguard TCC
Inchi:	InChI=1S/C13H9Cl3N2O/c14-8-1-3-9(4-2-8)17-13(19)18-10-5-6-11(15)12(16)7-10/h1-7H
InchiKey:	ICUTUKXCWQYESQ-UHFFFAOYSA-N
Formula:	C13H9Cl3N2O
SMILES:	O=C(Nc1ccc(Cl)cc1)Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	315.58
CAS:	101-20-2

Physical Properties

Property code	Value	Unit	Source
gf	268.58	kJ/mol	Joback Method
hf	74.14	kJ/mol	Joback Method
hfus	40.73	kJ/mol	Joback Method
hsub	182.20 ± 1.70	kJ/mol	NIST Webbook
hvap	83.84	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	5.291		Crippen Method
mcvol	204.760	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method

tb	831.64	K	Joback Method
tc	1085.50	K	Joback Method
tf	571.68	K	Joback Method
vc	0.770	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.73	J/mol×K	831.64	Joback Method
cpg	508.31	J/mol×K	873.95	Joback Method
cpg	516.93	J/mol×K	916.26	Joback Method
cpg	524.67	J/mol×K	958.57	Joback Method
cpg	531.59	J/mol×K	1000.88	Joback Method
cpg	537.76	J/mol×K	1043.19	Joback Method
cpg	543.26	J/mol×K	1085.50	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=C101202&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
hsub:	Enthalpy of sublimation 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

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