Urea, N-(4-chlorophenyl)-N'-(3,4-dichlorophenyl)-

Other names: 1-(3',4'-Dichlorophenyl)-3-(4'-chlorophenyl)urea
1-(4-Chlorophenyl)-3-(3,4-dichlorophenyl)urea
3,4,4'-Trichlorocarbanilide
3,4,4'-Trichlorodiphenylurea
CP 78416
Carbanilide, 3,4,4'-trichloro-
Cusiter
Cutisan
ENT 26925
Genoface
N-(3,4-Dichlorophenyl)-N'-(4-chlorophenyl)urea
N-(4-chlorophenyl)-N'-(3,4-dichlorophenyl)urea
NSC-72005
Nipaguard TCC
Procutene
Solubacter
TCC
Trilocarban

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]: 315.59

Physical Properties

Property code	Value	Unit	Source
hf	-87.77	kJ/mol	Cheméo Relay (1.0)
hfus	6.10	kJ/mol	Energetic studies of urea derivatives: Standard molar enthalpy of formation of 3,4,40-trichlorocarbanilide
hsub	182.20 ± 1.70	kJ/mol	NIST Webbook
hvap	118.86	kJ/mol	Cheméo Relay (1.0)
ie	7.80	eV	Cheméo Relay (1.0)
log10ws	-5.89		Cheméo Relay (1.0)
logp	5.291		Crippen Method
mcvol	204.760	ml/mol	McGowan Method

tb	637.74	K	Cheméo Relay (1.0)
tf	441.10	K	Cheméo Relay (1.0)

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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of climbazole and triclocarban in supercritical carbon dioxide: Measurement and correlation:	https://www.doi.org/10.1016/j.jct.2008.08.009
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101202&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Energetic studies of urea derivatives:	https://www.doi.org/10.1016/j.jct.2009.11.012
Standard molar enthalpy of formation of 3,4,4' trichlorocarbanilide:	
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point