N-(2,2,2-TRICHLORO-1,1-BIS(P-CHLOROPHENYL)

Other names: Acetamide, N-[2,2,2-trichloro-1,1-bis(4-chlorophenyl)ethyl]-
Acetamide, N-[1,1-bis(p-chlorophenyl)-2,2,2-trichloroethyl]-
N-[2,2,2-trichloro-1,1-bis(4-chlorophenyl)ethyl]acetamide
Inchi: InChI=1S/C16H12Cl5NO/c1-10(23)22-15(16(19,20)21,11-2-6-13(17)7-3-11)12-4-8-14(18
InchiKey: MCSLBZGLEIGWTI-UHFFFAOYSA-N
Formula: C16H12Cl5NO
SMILES: CC(=O)NC(c1ccc(Cl)cc1)(c1ccc(Cl)cc1)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 411.54

Physical Properties

Property code	Value	Unit	Source
hfus	37.35	kJ/mol	Joback Method
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-6.81		Cheméo Relay (1.0)
logp	5.743		Crippen Method
mcvol	261.530	ml/mol	McGowan Method
tb	657.55	K	Cheméo Relay (1.0)
tf	370.13	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.98	J/mol×K	913.53	Joback Method
cpg	663.63	J/mol×K	958.55	Joback Method
cpg	672.53	J/mol×K	1003.58	Joback Method
cpg	680.89	J/mol×K	1048.60	Joback Method
cpg	688.91	J/mol×K	1093.62	Joback Method
cpg	696.79	J/mol×K	1138.65	Joback Method
cpg	704.73	J/mol×K	1183.67	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81012955&Units=SI
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
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point