

N-(1,1-Bis(4-chlorophenyl)-2,2,2-trichloroethyl)acetamide

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
CAS:	81012-95-5

Physical Properties

Property code	Value	Unit	Source
gf	195.90	kJ/mol	Joback Method
hf	-78.76	kJ/mol	Joback Method
hfus	37.35	kJ/mol	Joback Method
hvap	89.60	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	5.743		Crippen Method
mcvol	261.530	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
tb	913.53	K	Joback Method
tc	1183.67	K	Joback Method
tf	604.99	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81012955&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcpvol:	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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