

p-Dimethylaminobenzylidene-p-chlorophenylacet

Inchi:	InChI=1S/C17H15ClN2/c1-20(2)17-9-3-13(4-10-17)11-15(12-19)14-5-7-16(18)8-6-14/h3-
InchiKey:	JYSGNKFGNNTQNO-RVDMUPIBSA-N
Formula:	C17H15ClN2
SMILES:	CN(C)c1ccc(C=C(C#N)c2ccc(Cl)cc2)cc1
Mol. weight [g/mol]:	282.77
CAS:	2958-46-5

Physical Properties

Property code	Value	Unit	Source
gf	601.52	kJ/mol	Joback Method
hf	380.01	kJ/mol	Joback Method
hfus	34.71	kJ/mol	Joback Method
hvap	76.26	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.470		Crippen Method
mcvol	222.170	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
tb	807.67	K	Joback Method
tc	1057.23	K	Joback Method
tf	467.57	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.12	J/molxK	807.67	Joback Method
cpg	604.50	J/molxK	849.26	Joback Method
cpg	616.84	J/molxK	890.86	Joback Method
cpg	628.26	J/molxK	932.45	Joback Method
cpg	638.89	J/molxK	974.04	Joback Method
cpg	648.84	J/molxK	1015.63	Joback Method
cpg	658.24	J/molxK	1057.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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/inchi/InChI%3D1S/C17H15CIN2/c1-20(2)17-9-3-13(4-10-17)11-15

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
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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