

o-Nitrobenzylidene-p-chlorophenylacetonitrile

Inchi:	InChI=1S/C15H9ClN2O2/c16-14-7-5-11(6-8-14)13(10-17)9-12-3-1-2-4-15(12)18(19)20/h
InchiKey:	LQKLMLDWVMTZPW-UKTHLTGXSA-N
Formula:	C15H9ClN2O2
SMILES:	N#CC(=Cc1ccccc1[N+](=O)[O-])c1ccc(Cl)cc1
Mol. weight [g/mol]:	284.70
CAS:	104089-71-6

Physical Properties

Property code	Value	Unit	Source
gf	509.45	kJ/mol	Joback Method
hf	343.00	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	86.35	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.312		Crippen Method
mcvol	201.430	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
tb	901.31	K	Joback Method
tc	1180.80	K	Joback Method
tf	556.17	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.24	J/molxK	901.31	Joback Method
cpg	540.12	J/molxK	947.89	Joback Method
cpg	549.16	J/molxK	994.47	Joback Method
cpg	557.53	J/molxK	1041.05	Joback Method
cpg	565.35	J/molxK	1087.63	Joback Method
cpg	572.78	J/molxK	1134.22	Joback Method
cpg	579.96	J/molxK	1180.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/inchi/InChI%3D1S/C15H9ClN2O2/c16-14-7-5-11(6-8-14)13(10-17)2
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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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