Procymidone

Other names:	1,2-Cyclopropanedicarboximide, N-(3,5-dichlorophenyl)-1,2-dimethyl- 3-(3,5-Dichlorophenyl)-1,5-dimethyl-3-azabicyclo[3.1.0]hexane-2,4-dione 3-(3,5-Dichlorophenyl)-1,5-dimethyl-3-azabicyclo[3.1.0]hexanedione 3-Azabicyclo[3.1.0]hexane-2,4-dione, 3-(3,5-dichlorophenyl)-1,5-dimethyl- Dicyclidine S 7131 Sumilex
Inchi:	InChI=1S/C13H11Cl2NO2/c1-12-6-13(12,2)11(18)16(10(12)17)9-4-7(14)3-8(15)5-9/h3-5
InchiKey:	QXJKBPAVAHBARF-UHFFFAOYSA-N
Formula:	C14H11Cl2NO2
SMILES:	CC12CC1(C)C(=O)N(c1cc(Cl)cc(Cl)c1)C2=O
Mol. weight [g/mol]:	296.15
CAS:	32809-16-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.80		Estimated Solubility Method
logp	3.283		Crippen Method
mcvol	186.150	ml/mol	McGowan Method
rinpol	2088.00		NIST Webbook
rinpol	2076.00		NIST Webbook
rinpol	2084.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2078.00		NIST Webbook
rinpol	2078.00		NIST Webbook
rinpol	2076.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2078.00		NIST Webbook
ripol	3032.00		NIST Webbook
ripol	3032.00		NIST Webbook
tf	438.40 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	30.09	kJ/mol	438.20	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32809168&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point