Fumaric acid, monoamide, N-methyl-N-phenyl-, 2,5-dichlorophenyl ester

Inchi: InChI=1S/C17H13Cl2NO3/c1-20(13-5-3-2-4-6-13)16(21)9-10-17(22)23-15-11-12(18)7-8-

InchiKey: KKVMLYZFPFFMRF-MDZDMXLPSA-N

Formula: C17H13Cl2NO3

SMILES: CN(C(=O)C=CC(=O)Oc1cc(Cl)ccc1Cl)c1ccccc1

Mol. weight [g/mol]: 350.20

Physical Properties

Property code	Value	Unit	Source
gf	102.12	kJ/mol	Joback Method
hf	-148.20	kJ/mol	Joback Method
hfus	43.09	kJ/mol	Joback Method
hvap	85.98	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.118		Crippen Method
mcvol	242.040	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	2786.00		NIST Webbook
rinpol	2786.00		NIST Webbook
tb	873.30	K	Joback Method
tc	1118.11	K	Joback Method
tf	568.55	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.58	J/mol×K	873.30	Joback Method
cpg	653.67	J/mol×K	914.10	Joback Method
cpg	663.73	J/mol×K	954.90	Joback Method
cpg	672.86	J/mol×K	995.71	Joback Method
cpg	681.14	J/mol×K	1036.51	Joback Method
cpg	688.66	J/mol×K	1077.31	Joback Method
cpg	695.52	J/mol×K	1118.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357470&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume