Fumaric acid, monoamide, N-methyl-N-phenyl-, 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C17H12Cl3NO3/c1-21(12-5-3-2-4-6-12)15(22)7-8-16(23)24-17-13(19)9-11(18)10-14(17)20/h2-10H,1H3/b8-7+

InchiKey: IPLQFONTBKNXRE-BQYQJAHWSA-N

Formula: C17H12Cl3NO3

SMILES: CN(C(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)c1ccccc1

Mol. weight [g/mol]: 384.64

Physical Properties

Property code	Value	Unit	Source
gf	80.56	kJ/mol	Joback Method
hf	-175.41	kJ/mol	Joback Method
hfus	46.90	kJ/mol	Joback Method
hvap	91.03	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.771		Crippen Method
mcvol	254.280	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	2894.00		NIST Webbook
rinpol	2894.00		NIST Webbook
tb	915.71	K	Joback Method
tc	1163.47	K	Joback Method
tf	610.99	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.92	J/mol×K	915.71	Joback Method
cpg	669.76	J/mol×K	957.00	Joback Method
cpg	678.65	J/mol×K	998.30	Joback Method
cpg	686.68	J/mol×K	1039.59	Joback Method
cpg	693.93	J/mol×K	1080.88	Joback Method
cpg	700.48	J/mol×K	1122.18	Joback Method
cpg	706.44	J/mol×K	1163.47	Joback Method

Sources

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/cbook.cgi?ID=U357465&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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