Fumaric acid, monoamide, N-(5-chloro-2-methoxyphenyl)-, 2,4,6-trichlorophenyl ester

InchiKey: BWKGQZJRDYDHNL-SNAWJCMRSA-N

Formula: C17H11Cl4NO4

SMILES: COc1ccc(Cl)cc1NC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 435.09

Physical Properties

Property code	Value	Unit	Source
gf	-77.02	kJ/mol	Joback Method
hf	-360.37	kJ/mol	Joback Method
hfus	53.59	kJ/mol	Joback Method
hvap	103.54	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.409		Crippen Method
mcvol	272.390	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	3500.00		NIST Webbook
tb	1023.25	K	Joback Method
tc	1275.38	K	Joback Method
tf	708.37	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.80	J/mol×K	1023.25	Joback Method
cpg	709.59	J/mol×K	1065.27	Joback Method
cpg	715.27	J/mol×K	1107.29	Joback Method
cpg	719.87	J/mol×K	1149.31	Joback Method
cpg	723.43	J/mol×K	1191.34	Joback Method
cpg	726.00	J/mol×K	1233.36	Joback Method
cpg	727.60	J/mol×K	1275.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357468&Units=SI

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