Fumaric acid, monoamide, N-(5-chloro-2-methoxyphenyl)-, 2-chlorophenyl ester

Inchi: InChI=1S/C17H13Cl2NO4/c1-23-15-7-6-11(18)10-13(15)20-16(21)8-9-17(22)24-14-5-3-2
InchiKey: PXGYZBRSISBTHA-CMDGGOBGSA-N
Formula: C17H13Cl2NO4
SMILES: COc1ccc(Cl)cc1NC(=O)C=CC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]: 366.19

Physical Properties

Property code	Value	Unit	Source
gf	-33.90	kJ/mol	Joback Method
hf	-305.95	kJ/mol	Joback Method
hfus	45.97	kJ/mol	Joback Method
hvap	93.45	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.102		Crippen Method
mcvol	247.910	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	3239.00		NIST Webbook
rinpol	3239.00		NIST Webbook
tb	938.43	K	Joback Method
tc	1183.07	K	Joback Method
tf	623.49	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.22	J/mol×K	938.43	Joback Method
cpg	683.69	J/mol×K	979.20	Joback Method
cpg	692.05	J/mol×K	1019.98	Joback Method
cpg	699.33	J/mol×K	1060.75	Joback Method
cpg	705.59	J/mol×K	1101.53	Joback Method
cpg	710.87	J/mol×K	1142.30	Joback Method
cpg	715.23	J/mol×K	1183.07	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=U357428&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