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

Inchi: InChI=1S/C18H15Cl2NO4/c1-11-9-12(19)3-5-15(11)25-18(23)8-7-17(22)21-14-10-13(20)
InchiKey: BKSXDXPWGLCLAS-BQYQJAHWSA-N
Formula: C18H15Cl2NO4
SMILES: COc1ccc(Cl)cc1NC(=O)C=CC(=O)Oc1ccc(Cl)cc1C
Mol. weight [g/mol]: 380.22

Physical Properties

Property code	Value	Unit	Source
gf	-35.11	kJ/mol	Joback Method
hf	-338.06	kJ/mol	Joback Method
hfus	48.17	kJ/mol	Joback Method
hvap	96.34	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.411		Crippen Method
mcvol	262.000	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	3347.00		NIST Webbook
rinpol	3347.00		NIST Webbook
tb	966.29	K	Joback Method
tc	1209.36	K	Joback Method
tf	647.28	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.60	J/mol×K	966.29	Joback Method
cpg	738.16	J/mol×K	1006.80	Joback Method
cpg	746.57	J/mol×K	1047.31	Joback Method
cpg	753.85	J/mol×K	1087.82	Joback Method
cpg	760.06	J/mol×K	1128.34	Joback Method
cpg	765.23	J/mol×K	1168.85	Joback Method
cpg	769.40	J/mol×K	1209.36	Joback Method

Sources

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=U357476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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