Fumaric acid, monoamide, N-(5-chloro-2-methoxyphenyl)-, 3,5-difluorophenyl ester

Other names: Fumaric acid, monoamide, N-(5-chloro-2-methoxyphenyl)-, 3,5-fluorophenyl ester
Inchi: InChI=1S/C17H12ClF2NO4/c1-24-15-3-2-10(18)6-14(15)21-16(22)4-5-17(23)25-13-8-11(
InchiKey: NULCGJZYDRWFCK-SNAWJCMRSA-N
Formula: C17H12ClF2NO4
SMILES: COc1ccc(Cl)cc1NC(=O)C=CC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 367.73

Physical Properties

Property code	Value	Unit	Source
gf	-421.22	kJ/mol	Joback Method
hf	-693.90	kJ/mol	Joback Method
hfus	47.54	kJ/mol	Joback Method
hvap	88.09	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.727		Crippen Method
mcvol	239.210	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	2936.00		NIST Webbook
tb	904.52	K	Joback Method
tc	1132.97	K	Joback Method
tf	607.27	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.32	J/mol×K	904.52	Joback Method
cpg	678.11	J/mol×K	942.59	Joback Method
cpg	686.87	J/mol×K	980.67	Joback Method
cpg	694.61	J/mol×K	1018.74	Joback Method
cpg	701.37	J/mol×K	1056.82	Joback Method
cpg	707.19	J/mol×K	1094.89	Joback Method
cpg	712.09	J/mol×K	1132.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357410&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