Fumaric acid, monoamide, N-(2-fluorophenyl)-, 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C16H9Cl3FNO3/c17-9-7-10(18)16(11(19)8-9)24-15(23)6-5-14(22)21-13-4-2-1-
InchiKey: HTNXBKUIHRNGDU-AATRIKPKSA-N
Formula: C16H9Cl3FNO3
SMILES: O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Nc1ccccc1F
Mol. weight [g/mol]: 388.61

Physical Properties

Property code	Value	Unit	Source
gf	-153.69	kJ/mol	Joback Method
hf	-376.41	kJ/mol	Joback Method
hfus	49.08	kJ/mol	Joback Method
hvap	93.04	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.886		Crippen Method
mcvol	241.960	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	2951.00		NIST Webbook
rinpol	2951.00		NIST Webbook
tb	934.81	K	Joback Method
tc	1179.99	K	Joback Method
tf	633.02	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.63	J/mol×K	934.81	Joback Method
cpg	625.84	J/mol×K	975.67	Joback Method
cpg	633.16	J/mol×K	1016.54	Joback Method
cpg	639.64	J/mol×K	1057.40	Joback Method
cpg	645.34	J/mol×K	1098.26	Joback Method
cpg	650.33	J/mol×K	1139.12	Joback Method
cpg	654.67	J/mol×K	1179.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357466&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

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