Fumaric acid, monoamide, N-(2-fluorophenyl)-, 2,5-dichlorophenyl ester

Inchi: InChI=1S/C16H10Cl2FNO3/c17-10-5-6-11(18)14(9-10)23-16(22)8-7-15(21)20-13-4-2-1-3

InchiKey: HFXBTJXSWXVERD-BQYQJAHWSA-N

Formula: C16H10Cl2FNO3

SMILES: O=C(C=CC(=O)Oc1cc(Cl)ccc1Cl)Nc1ccccc1F

Mol. weight [g/mol]: 354.16

Physical Properties

Property code	Value	Unit	Source
gf	-132.13	kJ/mol	Joback Method
hf	-349.20	kJ/mol	Joback Method
hfus	45.27	kJ/mol	Joback Method
hvap	88.00	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.233		Crippen Method
mcvol	229.720	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	2849.00		NIST Webbook
rinpol	2849.00		NIST Webbook
tb	892.40	K	Joback Method
tc	1134.30	K	Joback Method
tf	590.58	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.08	J/mol×K	892.40	Joback Method
cpg	611.47	J/mol×K	932.72	Joback Method
cpg	619.92	J/mol×K	973.03	Joback Method
cpg	627.48	J/mol×K	1013.35	Joback Method
cpg	634.24	J/mol×K	1053.67	Joback Method
cpg	640.24	J/mol×K	1093.99	Joback Method
cpg	645.56	J/mol×K	1134.30	Joback Method

Sources

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=U357471&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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