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

Other names: Fumaric acid, monoamide, N-(2-fluorophenyl)-, 3,5-fluorophenyl ester
Inchi: InChI=1S/C16H10F3NO3/c17-10-7-11(18)9-12(8-10)23-16(22)6-5-15(21)20-14-4-2-1-3-1
InchiKey: ZAPGXAMCOLOTES-AATRIKPKSA-N
Formula: C16H10F3NO3
SMILES: O=C(C=CC(=O)Oc1cc(F)cc(F)c1)Nc1ccccc1F
Mol. weight [g/mol]: 321.25

Physical Properties

Property code	Value	Unit	Source
gf	-497.89	kJ/mol	Joback Method
hf	-709.94	kJ/mol	Joback Method
hfus	43.04	kJ/mol	Joback Method
hvap	77.59	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.204		Crippen Method
mcvol	208.780	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	2402.00		NIST Webbook
rinpol	2402.00		NIST Webbook
tb	816.08	K	Joback Method
tc	1036.75	K	Joback Method
tf	531.92	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.70	J/mol×K	816.08	Joback Method
cpg	588.43	J/mol×K	852.86	Joback Method
cpg	598.24	J/mol×K	889.64	Joback Method
cpg	607.19	J/mol×K	926.41	Joback Method
cpg	615.32	J/mol×K	963.19	Joback Method
cpg	622.66	J/mol×K	999.97	Joback Method
cpg	629.29	J/mol×K	1036.75	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=U357406&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