Fumaric acid, monoamide, N-(4-chlorophenyl)-, 3,5-difluorophenyl ester

Other names: Fumaric acid, monoamide, N-(4-chlorophenyl)-, 3,5-fluorophenyl ester
Inchi: InChI=1S/C16H10ClF2NO3/c17-10-1-3-13(4-2-10)20-15(21)5-6-16(22)23-14-8-11(18)7-1
InchiKey: HFAUZDHXXZHRQK-AATRIKPKSA-N
Formula: C16H10ClF2NO3
SMILES: O=C(C=CC(=O)Oc1cc(F)cc(F)c1)Nc1ccc(Cl)cc1
Mol. weight [g/mol]: 337.70

Physical Properties

Property code	Value	Unit	Source
gf	-315.01	kJ/mol	Joback Method
hf	-529.57	kJ/mol	Joback Method
hfus	44.15	kJ/mol	Joback Method
hvap	82.80	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	3.718		Crippen Method
mcvol	219.250	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	2812.00		NIST Webbook
tb	854.24	K	Joback Method
tc	1085.51	K	Joback Method
tf	561.25	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.54	J/mol×K	854.24	Joback Method
cpg	600.61	J/mol×K	892.79	Joback Method
cpg	609.74	J/mol×K	931.33	Joback Method
cpg	618.00	J/mol×K	969.88	Joback Method
cpg	625.43	J/mol×K	1008.42	Joback Method
cpg	632.08	J/mol×K	1046.97	Joback Method
cpg	638.03	J/mol×K	1085.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357409&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