Fumaric acid, monoamide, N,N-dimethyl-, 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C12H10Cl3NO3/c1-16(2)10(17)3-4-11(18)19-12-8(14)5-7(13)6-9(12)15/h3-6H,

InchiKey: JQXLRBBRLNPXJP-ONEGZZNKSA-N

Formula: C12H10Cl3NO3

SMILES: CN(C)C(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 322.57

Physical Properties

Property code	Value	Unit	Source
gf	-73.95	kJ/mol	Joback Method
hf	-308.74	kJ/mol	Joback Method
hfus	39.91	kJ/mol	Joback Method
hvap	77.63	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.197		Crippen Method
mcvol	207.590	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	2437.00		NIST Webbook
rinpol	2437.00		NIST Webbook
tb	774.63	K	Joback Method
tc	1004.53	K	Joback Method
tf	528.22	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.98	J/mol×K	774.63	Joback Method
cpg	501.90	J/mol×K	812.95	Joback Method
cpg	511.01	J/mol×K	851.26	Joback Method
cpg	519.37	J/mol×K	889.58	Joback Method
cpg	527.00	J/mol×K	927.90	Joback Method
cpg	533.96	J/mol×K	966.21	Joback Method
cpg	540.29	J/mol×K	1004.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357463&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