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

Inchi: InChI=1S/C13H10Cl3NO3/c1-2-5-17-11(18)3-4-12(19)20-13-9(15)6-8(14)7-10(13)16/h2-4

InchiKey: DFLOCRBWCZQWAR-ONEGZZNKSA-N

Formula: C13H10Cl3NO3

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

Mol. weight [g/mol]: 334.58

Physical Properties

Property code	Value	Unit	Source
gf	0.92	kJ/mol	Joback Method
hf	-218.01	kJ/mol	Joback Method
hfus	43.30	kJ/mol	Joback Method
hvap	83.58	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.411		Crippen Method
mcvol	217.380	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	2559.00		NIST Webbook
tb	831.92	K	Joback Method
tc	1063.65	K	Joback Method
tf	557.92	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.94	J/mol×K	831.92	Joback Method
cpg	536.12	J/mol×K	870.54	Joback Method
cpg	544.53	J/mol×K	909.16	Joback Method
cpg	552.21	J/mol×K	947.79	Joback Method
cpg	559.20	J/mol×K	986.41	Joback Method
cpg	565.56	J/mol×K	1025.03	Joback Method
cpg	571.31	J/mol×K	1063.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357464&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

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