Fumaric acid, monoamide, N-(4-chlorophenyl)-, 2-chlorophenyl ester

Inchi: InChI=1S/C16H11Cl2NO3/c17-11-5-7-12(8-6-11)19-15(20)9-10-16(21)22-14-4-2-1-3-13(

InchiKey: HVQGQWQVWKBDDJ-MDZDMXLPSA-N

Formula: C16H11Cl2NO3

SMILES: O=C(C=CC(=O)Oc1ccccc1Cl)Nc1ccc(Cl)cc1

Mol. weight [g/mol]: 336.17

Physical Properties

Property code	Value	Unit	Source
gf	72.31	kJ/mol	Joback Method
hf	-141.62	kJ/mol	Joback Method
hfus	42.58	kJ/mol	Joback Method
hvap	88.15	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.094		Crippen Method
mcvol	227.950	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	3103.00		NIST Webbook
tb	888.15	K	Joback Method
tc	1137.96	K	Joback Method
tf	577.47	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.59	J/mol×K	888.15	Joback Method
cpg	606.52	J/mol×K	929.78	Joback Method
cpg	615.45	J/mol×K	971.42	Joback Method
cpg	623.46	J/mol×K	1013.05	Joback Method
cpg	630.63	J/mol×K	1054.69	Joback Method
cpg	637.04	J/mol×K	1096.32	Joback Method
cpg	642.77	J/mol×K	1137.96	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=U357427&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