Fumaric acid, monoamide, N-(2-ethylphenyl)-, 4-chloro-2-methylphenyl ester

Inchi: InChI=1S/C19H18ClNO3/c1-3-14-6-4-5-7-16(14)21-18(22)10-11-19(23)24-17-9-8-15(20)12-13(17)2/h4-12H,3H2,1-2H3,(H,21,22)/b11-10+

InchiKey: ZNQKRUXQBCNWHG-ZHACJKMWSA-N

Formula: C19H18ClNO3

SMILES: CCc1ccccc1NC(=O)C=CC(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 343.80

Physical Properties

Property code	Value	Unit	Source
gf	99.87	kJ/mol	Joback Method
hf	-199.27	kJ/mol	Joback Method
hfus	45.76	kJ/mol	Joback Method
hvap	91.11	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.311		Crippen Method
mcvol	257.980	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	3012.00		NIST Webbook
rinpol	3012.00		NIST Webbook
tb	924.34	K	Joback Method
tc	1162.79	K	Joback Method
tf	593.88	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.84	J/mol×K	924.34	Joback Method
cpg	754.70	J/mol×K	964.08	Joback Method
cpg	765.49	J/mol×K	1003.82	Joback Method
cpg	775.28	J/mol×K	1043.57	Joback Method
cpg	784.14	J/mol×K	1083.31	Joback Method
cpg	792.12	J/mol×K	1123.05	Joback Method
cpg	799.32	J/mol×K	1162.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357474&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