Fumaric acid, monoamide, N-methyl-N-phenyl-, 4-chloro-2-methylphenyl ester

Inchi: InChI=1S/C18H16ClNO3/c1-13-12-14(19)8-9-16(13)23-18(22)11-10-17(21)20(2)15-6-4-3
InchiKey: SNROMINFIHECEK-ZHACJKMWSA-N
Formula: C18H16ClNO3
SMILES: Cc1cc(Cl)ccc1OC(=O)C=CC(=O)N(C)c1ccccc1
Mol. weight [g/mol]: 329.78

Physical Properties

Property code	Value	Unit	Source
gf	122.47	kJ/mol	Joback Method
hf	-153.10	kJ/mol	Joback Method
hfus	41.49	kJ/mol	Joback Method
hvap	83.83	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.773		Crippen Method
mcvol	243.890	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	2753.00		NIST Webbook
tb	858.75	K	Joback Method
tc	1097.59	K	Joback Method
tf	549.90	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.08	J/mol×K	858.75	Joback Method
cpg	689.70	J/mol×K	898.56	Joback Method
cpg	701.21	J/mol×K	938.36	Joback Method
cpg	711.72	J/mol×K	978.17	Joback Method
cpg	721.31	J/mol×K	1017.98	Joback Method
cpg	730.06	J/mol×K	1057.78	Joback Method
cpg	738.05	J/mol×K	1097.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357473&Units=SI

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

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