Fumaric acid, monoamide, N,N-dimethyl-, 3-chlorophenyl ester

Inchi: InChI=1S/C12H12ClNO3/c1-14(2)11(15)6-7-12(16)17-10-5-3-4-9(13)8-10/h3-8H,1-2H3/b

InchiKey: DCBNHWNJXQUEEA-VOTSOKGWSA-N

Formula: C12H12ClNO3

SMILES: CN(C)C(=O)C=CC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 253.68

Physical Properties

Property code	Value	Unit	Source
gf	-30.83	kJ/mol	Joback Method
hf	-254.32	kJ/mol	Joback Method
hfus	32.29	kJ/mol	Joback Method
hvap	67.53	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.890		Crippen Method
mcvol	183.110	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	2202.00		NIST Webbook
tb	689.81	K	Joback Method
tc	912.63	K	Joback Method
tf	443.34	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.37	J/mol×K	689.81	Joback Method
cpg	463.63	J/mol×K	726.95	Joback Method
cpg	474.99	J/mol×K	764.08	Joback Method
cpg	485.49	J/mol×K	801.22	Joback Method
cpg	495.19	J/mol×K	838.36	Joback Method
cpg	504.12	J/mol×K	875.50	Joback Method
cpg	512.33	J/mol×K	912.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357444&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