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

Inchi: InChI=1S/C13H14ClNO3/c1-9(2)18-13(17)8-7-12(16)15-11-5-3-10(14)4-6-11/h3-9H,1-2H

InchiKey: JLNQFQCOGXLTRZ-BQYQJAHWSA-N

Formula: C13H14ClNO3

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

Mol. weight [g/mol]: 267.71

Physical Properties

Property code	Value	Unit	Source
gf	-46.24	kJ/mol	Joback Method
hf	-294.30	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	73.76	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.786		Crippen Method
mcvol	197.200	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinpol	2368.00		NIST Webbook
rinpol	2368.00		NIST Webbook
tb	749.98	K	Joback Method
tc	974.85	K	Joback Method
tf	459.80	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.63	J/mol×K	749.98	Joback Method
cpg	526.88	J/mol×K	787.46	Joback Method
cpg	538.20	J/mol×K	824.94	Joback Method
cpg	548.65	J/mol×K	862.42	Joback Method
cpg	558.25	J/mol×K	899.90	Joback Method
cpg	567.05	J/mol×K	937.37	Joback Method
cpg	575.10	J/mol×K	974.85	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=U357525&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