Fumaric acid, monoamide, N-(5-chloro-2-methoxyphenyl)-, isopropyl ester

Inchi: InChI=1S/C14H16ClNO4/c1-9(2)20-14(18)7-6-13(17)16-11-8-10(15)4-5-12(11)19-3/h4-9
InchiKey: CDLYVQUQMMALKU-VOTSOKGWSA-N
Formula: C14H16ClNO4
SMILES: COc1ccc(Cl)cc1NC(=O)C=CC(=O)OC(C)C
Mol. weight [g/mol]: 297.73

Physical Properties

Property code	Value	Unit	Source
gf	-152.45	kJ/mol	Joback Method
hf	-458.63	kJ/mol	Joback Method
hfus	36.83	kJ/mol	Joback Method
hvap	79.06	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.795		Crippen Method
mcvol	217.160	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	2507.00		NIST Webbook
tb	800.26	K	Joback Method
tc	1020.63	K	Joback Method
tf	505.82	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.02	J/mol×K	800.26	Joback Method
cpg	604.24	J/mol×K	836.99	Joback Method
cpg	615.50	J/mol×K	873.72	Joback Method
cpg	625.81	J/mol×K	910.45	Joback Method
cpg	635.21	J/mol×K	947.18	Joback Method
cpg	643.70	J/mol×K	983.90	Joback Method
cpg	651.32	J/mol×K	1020.63	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=U357526&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