Fumaric acid, monoamide, N-(5-chloro-2-methoxyphenyl)-, 4-isopropoxyphenyl ester

Inchi: InChI=1S/C20H20ClNO5/c1-13(2)26-15-5-7-16(8-6-15)27-20(24)11-10-19(23)22-17-12-1
InchiKey: MDDFRWTXOGFFMH-ZHACJKMWSA-N
Formula: C20H20ClNO5
SMILES: COc1ccc(Cl)cc1NC(=O)C=CC(=O)Oc1ccc(OC(C)C)cc1
Mol. weight [g/mol]: 389.83

Physical Properties

Property code	Value	Unit	Source
gf	-104.15	kJ/mol	Joback Method
hf	-489.63	kJ/mol	Joback Method
hfus	47.21	kJ/mol	Joback Method
hvap	97.76	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.236		Crippen Method
mcvol	283.810	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpol	3299.00		NIST Webbook
tb	991.62	K	Joback Method
tc	1229.90	K	Joback Method
tf	634.61	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.34	J/mol×K	991.62	Joback Method
cpg	861.64	J/mol×K	1031.33	Joback Method
cpg	870.56	J/mol×K	1071.05	Joback Method
cpg	878.11	J/mol×K	1110.76	Joback Method
cpg	884.33	J/mol×K	1150.48	Joback Method
cpg	889.26	J/mol×K	1190.19	Joback Method
cpg	892.92	J/mol×K	1229.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357423&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