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

InChI: InChI=1S/C17H12BrClFNO4/c1-24-15-4-2-10(19)8-13(15)21-16(22)6-7-17(23)25-14-5-3-
InChIKey: QDOQKHFSYBGXTR-VOTSOKGWSA-N
Formula: C17H12BrClFNO4
SMILES: COc1ccc(Cl)cc1NC(=O)C=CC(=O)Oc1ccc(F)cc1Br
Mol. weight [g/mol]: 428.64

Physical Properties

Property code	Value	Unit	Source
gf	-212.09	kJ/mol	Joback Method
hf	-471.46	kJ/mol	Joback Method
hfus	49.75	kJ/mol	Joback Method
hvap	95.34	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.350		Crippen Method
mcvol	254.940	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	3279.00		NIST Webbook
tb	971.41	K	Joback Method
tc	1215.85	K	Joback Method
tf	666.48	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.80	J/mol×K	971.41	Joback Method
cpg	695.36	J/mol×K	1012.15	Joback Method
cpg	702.91	J/mol×K	1052.89	Joback Method
cpg	709.48	J/mol×K	1093.63	Joback Method
cpg	715.12	J/mol×K	1134.37	Joback Method
cpg	719.90	J/mol×K	1175.11	Joback Method
cpg	723.85	J/mol×K	1215.85	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=U357419&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