Fumaric acid, monoamide, N-(2-bromophenyl)-, 4-chloro-2-methylphenyl ester

Inchi: InChI=1S/C17H13BrClNO3/c1-11-10-12(19)6-7-15(11)23-17(22)9-8-16(21)20-14-5-3-2-4
InchiKey: RJXNSHQGNMMVKI-CMDGGOBGSA-N
Formula: C17H13BrClNO3
SMILES: Cc1cc(Cl)ccc1OC(=O)C=CC(=O)Nc1ccccc1Br
Mol. weight [g/mol]: 394.65

Physical Properties

Property code	Value	Unit	Source
gf	97.35	kJ/mol	Joback Method
hf	-131.66	kJ/mol	Joback Method
hfus	45.87	kJ/mol	Joback Method
hvap	93.09	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	4.511		Crippen Method
mcvol	247.300	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
rinpol	3083.00		NIST Webbook
rinpol	3083.00		NIST Webbook
tb	944.74	K	Joback Method
tc	1197.82	K	Joback Method
tf	631.14	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.71	J/mol×K	944.74	Joback Method
cpg	667.54	J/mol×K	986.92	Joback Method
cpg	676.44	J/mol×K	1029.10	Joback Method
cpg	684.50	J/mol×K	1071.28	Joback Method
cpg	691.82	J/mol×K	1113.46	Joback Method
cpg	698.48	J/mol×K	1155.64	Joback Method
cpg	704.58	J/mol×K	1197.82	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=U357475&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