Fumaric acid, monoamide, N-(2-methoxy-5-chlorophenyl)-, 4-bromophenyl ester

InChI: InChI=1S/C17H13BrClNO4/c1-23-15-7-4-12(19)10-14(15)20-16(21)8-9-17(22)24-13-5-2-
InChIKey: JWRMBCKJMXXMEC-CMDGGOBGSA-N
Formula: C17H13BrClNO4
SMILES: COc1ccc(Cl)cc1NC(=O)C=CC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 410.65

Physical Properties

Property code	Value	Unit	Source
gf	-7.65	kJ/mol	Joback Method
hf	-263.88	kJ/mol	Joback Method
hfus	47.06	kJ/mol	Joback Method
hvap	95.50	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.211		Crippen Method
mcvol	253.170	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	3426.00		NIST Webbook
rinpol	3426.00		NIST Webbook
tb	967.16	K	Joback Method
tc	1217.98	K	Joback Method
tf	653.37	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.68	J/mol×K	967.16	Joback Method
cpg	690.74	J/mol×K	1008.96	Joback Method
cpg	698.75	J/mol×K	1050.77	Joback Method
cpg	705.77	J/mol×K	1092.57	Joback Method
cpg	711.85	J/mol×K	1134.38	Joback Method
cpg	717.07	J/mol×K	1176.18	Joback Method
cpg	721.49	J/mol×K	1217.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357436&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