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

Inchi: InChI=1S/C16H11BrClNO3/c17-11-5-1-3-7-13(11)19-15(20)9-10-16(21)22-14-8-4-2-6-12

InchiKey: ZVUREVVWAKOFDI-MDZDMXLPSA-N

Formula: C16H11BrClNO3

SMILES: O=C(C=CC(=O)Oc1ccccc1Cl)Nc1ccccc1Br

Mol. weight [g/mol]: 380.62

Physical Properties

Property code	Value	Unit	Source
gf	98.56	kJ/mol	Joback Method
hf	-99.55	kJ/mol	Joback Method
hfus	43.67	kJ/mol	Joback Method
hvap	90.20	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.203		Crippen Method
mcvol	233.210	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	2965.00		NIST Webbook
tb	916.88	K	Joback Method
tc	1173.17	K	Joback Method
tf	607.35	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.11	J/mol×K	916.88	Joback Method
cpg	613.66	J/mol×K	959.60	Joback Method
cpg	622.29	J/mol×K	1002.31	Joback Method
cpg	630.10	J/mol×K	1045.03	Joback Method
cpg	637.19	J/mol×K	1087.74	Joback Method
cpg	643.67	J/mol×K	1130.46	Joback Method
cpg	649.61	J/mol×K	1173.17	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=U357426&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