Fumaric acid, monoamide, N-(2-bromophenyl)-, 3-fluorophenyl ester

Inchi: InChI=1S/C16H11BrFNO3/c17-13-6-1-2-7-14(13)19-15(20)8-9-16(21)22-12-5-3-4-11(18)10-12/h1-10H,(H,19,20)/b9-8+

InchiKey: JQMXYAJTDHWLIV-CMDGGOBGSA-N

Formula: C16H11BrFNO3

SMILES: O=C(C=CC(=O)Oc1cccc(F)c1)Nc1ccccc1Br

Mol. weight [g/mol]: 364.17

Physical Properties

Property code	Value	Unit	Source
gf	-84.32	kJ/mol	Joback Method
hf	-279.92	kJ/mol	Joback Method
hfus	42.55	kJ/mol	Joback Method
hvap	85.00	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.688		Crippen Method
mcvol	222.740	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	2752.00		NIST Webbook
rinpol	2752.00		NIST Webbook
tb	878.72	K	Joback Method
tc	1124.02	K	Joback Method
tf	578.02	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.11	J/mol×K	878.72	Joback Method
cpg	603.29	J/mol×K	919.60	Joback Method
cpg	612.52	J/mol×K	960.49	Joback Method
cpg	620.91	J/mol×K	1001.37	Joback Method
cpg	628.52	J/mol×K	1042.26	Joback Method
cpg	635.45	J/mol×K	1083.14	Joback Method
cpg	641.77	J/mol×K	1124.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357488&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

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