Fumaric acid, monoamide, N-methyl-N-phenyl-, 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C17H13BrFNO3/c1-20(13-5-3-2-4-6-13)16(21)9-10-17(22)23-15-8-7-12(19)11-
InchiKey: BRFZUMBQKALODG-MDZDMXLPSA-N
Formula: C17H13BrFNO3
SMILES: CN(C(=O)C=CC(=O)Oc1ccc(F)cc1Br)c1ccccc1
Mol. weight [g/mol]: 378.19

Physical Properties

Property code	Value	Unit	Source
gf	-54.51	kJ/mol	Joback Method
hf	-286.50	kJ/mol	Joback Method
hfus	43.06	kJ/mol	Joback Method
hvap	82.83	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.713		Crippen Method
mcvol	236.830	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	2692.00		NIST Webbook
rinpol	2692.00		NIST Webbook
tb	863.87	K	Joback Method
tc	1104.24	K	Joback Method
tf	569.10	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.72	J/mol×K	863.87	Joback Method
cpg	650.03	J/mol×K	903.93	Joback Method
cpg	660.37	J/mol×K	943.99	Joback Method
cpg	669.83	J/mol×K	984.05	Joback Method
cpg	678.50	J/mol×K	1024.12	Joback Method
cpg	686.48	J/mol×K	1064.18	Joback Method
cpg	693.86	J/mol×K	1104.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357416&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