Fumaric acid, monoamide, N,N-dimethyl-, 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C12H11BrFNO3/c1-15(2)11(16)5-6-12(17)18-10-4-3-8(14)7-9(10)13/h3-7H,1-2

InchiKey: BSOWWZLHXYEGAG-AATRIKPKSA-N

Formula: C12H11BrFNO3

SMILES: CN(C)C(=O)C=CC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 316.12

Physical Properties

Property code	Value	Unit	Source
gf	-209.02	kJ/mol	Joback Method
hf	-419.83	kJ/mol	Joback Method
hfus	36.07	kJ/mol	Joback Method
hvap	69.43	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.138		Crippen Method
mcvol	190.140	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	2205.00		NIST Webbook
tb	722.79	K	Joback Method
tc	944.43	K	Joback Method
tf	486.33	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.21	J/mol×K	722.79	Joback Method
cpg	479.34	J/mol×K	759.73	Joback Method
cpg	489.66	J/mol×K	796.67	Joback Method
cpg	499.20	J/mol×K	833.61	Joback Method
cpg	508.02	J/mol×K	870.55	Joback Method
cpg	516.17	J/mol×K	907.49	Joback Method
cpg	523.70	J/mol×K	944.43	Joback Method

Sources

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=U357414&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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