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

Inchi: InChI=1S/C13H11BrFNO3/c1-2-7-16-12(17)5-6-13(18)19-11-4-3-9(15)8-10(11)14/h2-6,8

InchiKey: OMXQAJJJLBKDFL-AATRIKPKSA-N

Formula: C13H11BrFNO3

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

Mol. weight [g/mol]: 328.13

Physical Properties

Property code	Value	Unit	Source
gf	-134.15	kJ/mol	Joback Method
hf	-329.10	kJ/mol	Joback Method
hfus	39.46	kJ/mol	Joback Method
hvap	75.38	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	2.352		Crippen Method
mcvol	199.930	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	2336.00		NIST Webbook
rinpol	2336.00		NIST Webbook
tb	780.08	K	Joback Method
tc	1003.90	K	Joback Method
tf	516.03	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.02	J/mol×K	780.08	Joback Method
cpg	515.39	J/mol×K	817.38	Joback Method
cpg	524.99	J/mol×K	854.69	Joback Method
cpg	533.85	J/mol×K	891.99	Joback Method
cpg	542.04	J/mol×K	929.30	Joback Method
cpg	549.60	J/mol×K	966.60	Joback Method
cpg	556.59	J/mol×K	1003.90	Joback Method

Sources

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=U357415&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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