Fumaric acid, monoamide, N-(2-bromophenyl)-, 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C16H10Br2FNO3/c17-11-3-1-2-4-13(11)20-15(21)7-8-16(22)23-14-6-5-10(19)9
InchiKey: KVLLOGSQHBXDSA-BQYQJAHWSA-N
Formula: C16H10Br2FNO3
SMILES: O=C(C=CC(=O)Oc1ccc(F)cc1Br)Nc1ccccc1Br
Mol. weight [g/mol]: 443.06

Physical Properties

Property code	Value	Unit	Source
gf	-79.63	kJ/mol	Joback Method
hf	-265.06	kJ/mol	Joback Method
hfus	47.45	kJ/mol	Joback Method
hvap	92.10	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	4.451		Crippen Method
mcvol	240.240	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	3009.00		NIST Webbook
tb	949.86	K	Joback Method
tc	1204.41	K	Joback Method
tf	650.34	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.42	J/mol×K	949.86	Joback Method
cpg	625.16	J/mol×K	992.29	Joback Method
cpg	633.14	J/mol×K	1034.71	Joback Method
cpg	640.46	J/mol×K	1077.14	Joback Method
cpg	647.20	J/mol×K	1119.56	Joback Method
cpg	653.46	J/mol×K	1161.99	Joback Method
cpg	659.36	J/mol×K	1204.41	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=U357418&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