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

Inchi: InChI=1S/C19H18BrNO4/c1-13(2)24-14-7-9-15(10-8-14)25-19(23)12-11-18(22)21-17-6-4
InchiKey: MHGKFTLESWOHIN-VAWYXSNFSA-N
Formula: C19H18BrNO4
SMILES: CC(C)Oc1ccc(OC(=O)C=CC(=O)Nc2ccccc2Br)cc1
Mol. weight [g/mol]: 404.25

Physical Properties

Property code	Value	Unit	Source
gf	28.31	kJ/mol	Joback Method
hf	-283.23	kJ/mol	Joback Method
hfus	44.91	kJ/mol	Joback Method
hvap	94.52	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.337		Crippen Method
mcvol	269.110	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	3033.00		NIST Webbook
rinpol	3033.00		NIST Webbook
tb	970.07	K	Joback Method
tc	1215.53	K	Joback Method
tf	618.47	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.34	J/mol×K	970.07	Joback Method
cpg	790.17	J/mol×K	1010.98	Joback Method
cpg	799.87	J/mol×K	1051.89	Joback Method
cpg	808.51	J/mol×K	1092.80	Joback Method
cpg	816.16	J/mol×K	1133.71	Joback Method
cpg	822.89	J/mol×K	1174.62	Joback Method
cpg	828.77	J/mol×K	1215.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357422&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