Fumaric acid, monoamide, N-(2-bromophenyl)-, isopropyl ester

Inchi: InChI=1S/C13H14BrNO3/c1-9(2)18-13(17)8-7-12(16)15-11-6-4-3-5-10(11)14/h3-9H,1-2H

InchiKey: SAKFWXOMFJZLLW-BQYQJAHWSA-N

Formula: C13H14BrNO3

SMILES: CC(C)OC(=O)C=CC(=O)Nc1ccccc1Br

Mol. weight [g/mol]: 312.16

Physical Properties

Property code	Value	Unit	Source
gf	-19.99	kJ/mol	Joback Method
hf	-252.23	kJ/mol	Joback Method
hfus	34.53	kJ/mol	Joback Method
hvap	75.81	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.895		Crippen Method
mcvol	202.460	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	2228.00		NIST Webbook
rinpol	2228.00		NIST Webbook
tb	778.71	K	Joback Method
tc	1010.61	K	Joback Method
tf	489.68	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.78	J/mol×K	778.71	Joback Method
cpg	536.59	J/mol×K	817.36	Joback Method
cpg	547.47	J/mol×K	856.01	Joback Method
cpg	557.50	J/mol×K	894.66	Joback Method
cpg	566.72	J/mol×K	933.31	Joback Method
cpg	575.19	J/mol×K	971.96	Joback Method
cpg	582.97	J/mol×K	1010.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357524&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

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