Fumaric acid, monoamide, N,N-dimethyl-, 4-bromophenyl ester

Inchi: InChI=1S/C12H12BrNO3/c1-14(2)11(15)7-8-12(16)17-10-5-3-9(13)4-6-10/h3-8H,1-2H3/b

InchiKey: AXAWANFJJMMQAK-BQYQJAHWSA-N

Formula: C12H12BrNO3

SMILES: CN(C)C(=O)C=CC(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 298.13

Physical Properties

Property code	Value	Unit	Source
gf	-4.58	kJ/mol	Joback Method
hf	-212.25	kJ/mol	Joback Method
hfus	33.38	kJ/mol	Joback Method
hvap	69.58	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.999		Crippen Method
mcvol	188.370	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	2334.00		NIST Webbook
tb	718.54	K	Joback Method
tc	948.92	K	Joback Method
tf	473.22	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.78	J/mol×K	718.54	Joback Method
cpg	473.60	J/mol×K	756.94	Joback Method
cpg	484.52	J/mol×K	795.33	Joback Method
cpg	494.60	J/mol×K	833.73	Joback Method
cpg	503.88	J/mol×K	872.12	Joback Method
cpg	512.44	J/mol×K	910.52	Joback Method
cpg	520.34	J/mol×K	948.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357432&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