Fumaric acid, monoamide, N-methyl-N-phenyl-, 4-bromophenyl ester

Inchi: InChI=1S/C17H14BrNO3/c1-19(14-5-3-2-4-6-14)16(20)11-12-17(21)22-15-9-7-13(18)8-1

InchiKey: UKUMPJAFVXSDSP-VAWYXSNFSA-N

Formula: C17H14BrNO3

SMILES: CN(C(=O)C=CC(=O)Oc1ccc(Br)cc1)c1ccccc1

Mol. weight [g/mol]: 360.20

Physical Properties

Property code	Value	Unit	Source
gf	149.93	kJ/mol	Joback Method
hf	-78.92	kJ/mol	Joback Method
hfus	40.37	kJ/mol	Joback Method
hvap	82.99	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.574		Crippen Method
mcvol	235.060	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
rinpol	2805.00		NIST Webbook
rinpol	2805.00		NIST Webbook
tb	859.62	K	Joback Method
tc	1108.27	K	Joback Method
tf	555.99	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.91	J/mol×K	859.62	Joback Method
cpg	644.85	J/mol×K	901.06	Joback Method
cpg	655.75	J/mol×K	942.50	Joback Method
cpg	665.71	J/mol×K	983.95	Joback Method
cpg	674.85	J/mol×K	1025.39	Joback Method
cpg	683.28	J/mol×K	1066.83	Joback Method
cpg	691.12	J/mol×K	1108.27	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=U357434&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