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

Inchi: InChI=1S/C13H12BrNO3/c1-2-9-15-12(16)7-8-13(17)18-11-5-3-10(14)4-6-11/h2-8H,1,9H

InchiKey: KNHGDANWWLGUKN-BQYQJAHWSA-N

Formula: C13H12BrNO3

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

Mol. weight [g/mol]: 310.14

Physical Properties

Property code	Value	Unit	Source
gf	70.29	kJ/mol	Joback Method
hf	-121.52	kJ/mol	Joback Method
hfus	36.77	kJ/mol	Joback Method
hvap	75.53	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.213		Crippen Method
mcvol	198.160	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	2464.00		NIST Webbook
tb	775.83	K	Joback Method
tc	1007.71	K	Joback Method
tf	502.92	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.93	J/mol×K	775.83	Joback Method
cpg	509.91	J/mol×K	814.48	Joback Method
cpg	520.03	J/mol×K	853.12	Joback Method
cpg	529.36	J/mol×K	891.77	Joback Method
cpg	537.98	J/mol×K	930.42	Joback Method
cpg	545.92	J/mol×K	969.07	Joback Method
cpg	553.27	J/mol×K	1007.71	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357433&Units=SI

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