Fumaric acid, 4-bromophenyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C15H15BrO4/c1-11(2)9-10-19-14(17)7-8-15(18)20-13-5-3-12(16)4-6-13/h3-9H

InchiKey: GOEXWHDUBBXHRQ-BQYQJAHWSA-N

Formula: C15H15BrO4

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

Mol. weight [g/mol]: 339.18

Physical Properties

Property code	Value	Unit	Source
gf	-123.43	kJ/mol	Joback Method
hf	-366.49	kJ/mol	Joback Method
hfus	38.21	kJ/mol	Joback Method
hvap	76.67	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.420		Crippen Method
mcvol	222.230	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	2273.00		NIST Webbook
rinpol	2273.00		NIST Webbook
tb	801.20	K	Joback Method
tc	1031.78	K	Joback Method
tf	477.75	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.84	J/mol×K	801.20	Joback Method
cpg	592.13	J/mol×K	839.63	Joback Method
cpg	603.52	J/mol×K	878.06	Joback Method
cpg	614.06	J/mol×K	916.49	Joback Method
cpg	623.80	J/mol×K	954.92	Joback Method
cpg	632.81	J/mol×K	993.35	Joback Method
cpg	641.14	J/mol×K	1031.78	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=U405768&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