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

Inchi: InChI=1S/C15H17BrO4/c1-10(2)11(3)19-14(17)8-9-15(18)20-13-6-4-12(16)5-7-13/h4-11H

InchiKey: FKSBAJRHMLROJH-CMDGGOBGSA-N

Formula: C15H17BrO4

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

Mol. weight [g/mol]: 341.20

Physical Properties

Property code	Value	Unit	Source
gf	-199.98	kJ/mol	Joback Method
hf	-484.48	kJ/mol	Joback Method
hfus	32.27	kJ/mol	Joback Method
hvap	75.85	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.498		Crippen Method
mcvol	226.530	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
tb	796.28	K	Joback Method
tc	1023.66	K	Joback Method
tf	466.79	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.46	J/mol×K	796.28	Joback Method
cpg	620.53	J/mol×K	834.18	Joback Method
cpg	632.59	J/mol×K	872.07	Joback Method
cpg	643.65	J/mol×K	909.97	Joback Method
cpg	653.78	J/mol×K	947.86	Joback Method
cpg	662.99	J/mol×K	985.76	Joback Method
cpg	671.34	J/mol×K	1023.66	Joback Method
dvisc	0.0007626	Pa×s	466.79	Joback Method

dvisc	0.0004076	Pa×s	521.71	Joback Method
dvisc	0.0002455	Pa×s	576.62	Joback Method
dvisc	0.0001614	Pa×s	631.53	Joback Method
dvisc	0.0001135	Pa×s	686.45	Joback Method
dvisc	0.0000841	Pa×s	741.37	Joback Method
dvisc	0.0000650	Pa×s	796.28	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=U405766&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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