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

Inchi: InChI=1S/C16H19BrO4/c1-4-14(11(2)3)21-16(19)10-9-15(18)20-13-7-5-12(17)6-8-13/h5-

InchiKey: PQSLNALBKWVLOB-MDZDMXLPSA-N

Formula: C16H19BrO4

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

Mol. weight [g/mol]: 355.22

Physical Properties

Property code	Value	Unit	Source
gf	-191.56	kJ/mol	Joback Method
hf	-505.12	kJ/mol	Joback Method
hfus	34.86	kJ/mol	Joback Method
hvap	78.08	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.888		Crippen Method
mcvol	240.620	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	819.16	K	Joback Method
tc	1043.54	K	Joback Method
tf	478.06	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.43	J/mol×K	819.16	Joback Method
cpg	675.80	J/mol×K	856.56	Joback Method
cpg	688.14	J/mol×K	893.95	Joback Method
cpg	699.47	J/mol×K	931.35	Joback Method
cpg	709.85	J/mol×K	968.75	Joback Method
cpg	719.31	J/mol×K	1006.15	Joback Method
cpg	727.90	J/mol×K	1043.54	Joback Method
dvisc	0.0006886	Pa×s	478.06	Joback Method

dvisc	0.0003636	Pa×s	534.91	Joback Method
dvisc	0.0002171	Pa×s	591.76	Joback Method
dvisc	0.0001419	Pa×s	648.61	Joback Method
dvisc	0.0000993	Pa×s	705.46	Joback Method
dvisc	0.0000733	Pa×s	762.31	Joback Method
dvisc	0.0000564	Pa×s	819.16	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=U405767&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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