Fumaric acid, 4-bromophenyl 3-chlorophenyl ester

Inchi: InChI=1S/C16H10BrClO4/c17-11-4-6-13(7-5-11)21-15(19)8-9-16(20)22-14-3-1-2-12(18)1

InchiKey: DRLAOBSMEUYVDP-CMDGGOBGSA-N

Formula: C16H10BrClO4

SMILES: O=C(C=CC(=O)Oc1cccc(Cl)c1)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 381.61

Physical Properties

Property code	Value	Unit	Source
gf	-95.83	kJ/mol	Joback Method
hf	-285.24	kJ/mol	Joback Method
hfus	39.76	kJ/mol	Joback Method
hvap	86.18	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.170		Crippen Method
mcvol	229.100	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	2639.00		NIST Webbook
tb	889.13	K	Joback Method
tc	1144.89	K	Joback Method
tf	576.92	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.41	J/mol×K	889.13	Joback Method
cpg	618.97	J/mol×K	1102.27	Joback Method
cpg	613.11	J/mol×K	1059.64	Joback Method
cpg	606.39	J/mol×K	1017.01	Joback Method
cpg	598.74	J/mol×K	974.38	Joback Method
cpg	590.11	J/mol×K	931.76	Joback Method
cpg	624.05	J/mol×K	1144.89	Joback Method
dvisc	0.0000603	Pa×s	889.13	Joback Method
dvisc	0.0000742	Pa×s	837.10	Joback Method

dvisc	0.0000937	Pa×s	785.06	Joback Method
dvisc	0.0001223	Pa×s	733.03	Joback Method
dvisc	0.0001664	Pa×s	680.99	Joback Method
dvisc	0.0002381	Pa×s	628.96	Joback Method
dvisc	0.0003635	Pa×s	576.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405775&Units=SI
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

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