Fumaric acid, 4-bromophenyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C16H9BrClFO4/c17-10-4-6-11(7-5-10)22-14(20)8-9-15(21)23-16-12(18)2-1-3-1

InchiKey: VJNLWFLQDHCGFG-CMDGGOBGSA-N

Formula: C16H9BrClFO4

SMILES: O=C(C=CC(=O)Oc1c(F)cccc1Cl)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 399.60

Physical Properties

Property code	Value	Unit	Source
gf	-300.27	kJ/mol	Joback Method
hf	-492.82	kJ/mol	Joback Method
hfus	42.45	kJ/mol	Joback Method
hvap	86.02	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.309		Crippen Method
mcvol	230.870	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	2585.00		NIST Webbook
tb	893.38	K	Joback Method
tc	1140.67	K	Joback Method
tf	590.03	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.86	J/mol×K	893.38	Joback Method
cpg	595.00	J/mol×K	934.59	Joback Method
cpg	603.14	J/mol×K	975.81	Joback Method
cpg	610.34	J/mol×K	1017.02	Joback Method
cpg	616.65	J/mol×K	1058.24	Joback Method
cpg	622.12	J/mol×K	1099.45	Joback Method
cpg	626.80	J/mol×K	1140.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405774&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

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