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

Inchi: InChI=1S/C17H11Cl2FO4/c18-12-6-4-11(5-7-12)10-23-15(21)8-9-16(22)24-17-13(19)2-1

InchiKey: NANSSLAJRASVIG-CMDGGOBGSA-N

Formula: C17H11Cl2FO4

SMILES: O=C(C=CC(=O)Oc1c(F)cccc1Cl)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 369.17

Physical Properties

Property code	Value	Unit	Source
gf	-318.10	kJ/mol	Joback Method
hf	-555.53	kJ/mol	Joback Method
hfus	43.95	kJ/mol	Joback Method
hvap	86.20	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.337		Crippen Method
mcvol	239.700	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	2604.00		NIST Webbook
rinpol	2604.00		NIST Webbook
tb	887.53	K	Joback Method
tc	1125.09	K	Joback Method
tf	571.42	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.81	J/mol×K	887.53	Joback Method
cpg	642.73	J/mol×K	927.12	Joback Method
cpg	651.60	J/mol×K	966.72	Joback Method
cpg	659.46	J/mol×K	1006.31	Joback Method
cpg	666.34	J/mol×K	1045.91	Joback Method
cpg	672.30	J/mol×K	1085.50	Joback Method
cpg	677.37	J/mol×K	1125.09	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=U405921&Units=SI

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