Fumaric acid, 4-chlorobenzyl 2-fluorophenyl ester

Inchi: InChI=1S/C17H12ClFO4/c18-13-7-5-12(6-8-13)11-22-16(20)9-10-17(21)23-15-4-2-1-3-14

InchiKey: UULFQARRZLKFJE-MDZDMXLPSA-N

Formula: C17H12ClFO4

SMILES: O=C(C=CC(=O)Oc1ccccc1F)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 334.73

Physical Properties

Property code	Value	Unit	Source
gf	-296.54	kJ/mol	Joback Method
hf	-528.32	kJ/mol	Joback Method
hfus	40.14	kJ/mol	Joback Method
hvap	81.15	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.684		Crippen Method
mcvol	227.460	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	2469.00		NIST Webbook
rinpol	2469.00		NIST Webbook
tb	845.12	K	Joback Method
tc	1079.30	K	Joback Method
tf	528.98	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.60	J/mol×K	845.12	Joback Method
cpg	625.85	J/mol×K	884.15	Joback Method
cpg	636.02	J/mol×K	923.18	Joback Method
cpg	645.15	J/mol×K	962.21	Joback Method
cpg	653.29	J/mol×K	1001.24	Joback Method
cpg	660.48	J/mol×K	1040.27	Joback Method
cpg	666.77	J/mol×K	1079.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405918&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