Fumaric acid, 2-chlorophenyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C13H9ClF4O4/c14-8-3-1-2-4-9(8)22-11(20)6-5-10(19)21-7-13(17,18)12(15)16/

InchiKey: JINZRBSIVPZAEZ-AATRIKPKSA-N

Formula: C13H9ClF4O4

SMILES: O=C(C=CC(=O)Oc1ccccc1Cl)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 340.65

Physical Properties

Property code	Value	Unit	Source
gf	-1017.03	kJ/mol	Joback Method
hf	-1273.18	kJ/mol	Joback Method
hfus	34.43	kJ/mol	Joback Method
hvap	65.17	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.245		Crippen Method
mcvol	200.170	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	1777.00		NIST Webbook
rinpol	1777.00		NIST Webbook
tb	716.08	K	Joback Method
tc	916.69	K	Joback Method
tf	434.15	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.10	J/mol×K	716.08	Joback Method
cpg	534.73	J/mol×K	749.51	Joback Method
cpg	544.56	J/mol×K	782.95	Joback Method
cpg	553.63	J/mol×K	816.38	Joback Method
cpg	561.96	J/mol×K	849.82	Joback Method
cpg	569.61	J/mol×K	883.25	Joback Method
cpg	576.61	J/mol×K	916.69	Joback Method

Sources

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=U405718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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