Fumaric acid, 2,4,6-trichlorophenyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C13H7Cl3F4O4/c14-6-3-7(15)11(8(16)4-6)24-10(22)2-1-9(21)23-5-13(19,20)12

InchiKey: PXGGAIRITFBZQO-OWOJBTEDSA-N

Formula: C13H7Cl3F4O4

SMILES: O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 409.55

Physical Properties

Property code	Value	Unit	Source
gf	-1060.15	kJ/mol	Joback Method
hf	-1327.60	kJ/mol	Joback Method
hfus	42.05	kJ/mol	Joback Method
hvap	75.27	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.552		Crippen Method
mcvol	224.650	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	2020.00		NIST Webbook
rinpol	2020.00		NIST Webbook
tb	800.90	K	Joback Method
tc	1010.48	K	Joback Method
tf	519.03	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.98	J/mol×K	800.90	Joback Method
cpg	571.44	J/mol×K	835.83	Joback Method
cpg	579.17	J/mol×K	870.76	Joback Method
cpg	586.19	J/mol×K	905.69	Joback Method
cpg	592.55	J/mol×K	940.62	Joback Method
cpg	598.27	J/mol×K	975.55	Joback Method
cpg	603.40	J/mol×K	1010.48	Joback Method

Sources

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=U405946&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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