Fumaric acid, 2,4,6-trichlorophenyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C15H7Cl3F8O4/c16-6-3-7(17)11(8(18)4-6)30-10(28)2-1-9(27)29-5-13(21,22)15

InchiKey: LKZFADVGKKDHAF-OWOJBTEDSA-N

Formula: C15H7Cl3F8O4

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

Mol. weight [g/mol]: 509.56

Physical Properties

Property code	Value	Unit	Source
gf	-1816.87	kJ/mol	Joback Method
hf	-2170.82	kJ/mol	Joback Method
hfus	44.72	kJ/mol	Joback Method
hvap	73.86	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.823		Crippen Method
mcvol	259.910	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	2117.00		NIST Webbook
tb	837.28	K	Joback Method
tc	1037.21	K	Joback Method
tf	548.77	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.03	J/mol×K	837.28	Joback Method
cpg	711.04	J/mol×K	870.60	Joback Method
cpg	718.37	J/mol×K	903.92	Joback Method
cpg	725.09	J/mol×K	937.25	Joback Method
cpg	731.26	J/mol×K	970.57	Joback Method
cpg	736.96	J/mol×K	1003.89	Joback Method
cpg	742.27	J/mol×K	1037.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405947&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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