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

Inchi: InChI=1S/C15H8Cl2F8O4/c16-7-2-1-3-8(17)11(7)29-10(27)5-4-9(26)28-6-13(20,21)15(24

InchiKey: WDQJLWNBIAIJGJ-SNAWJCMRSA-N

Formula: C15H8Cl2F8O4

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

Mol. weight [g/mol]: 475.12

Physical Properties

Property code	Value	Unit	Source
gf	-1795.31	kJ/mol	Joback Method
hf	-2143.61	kJ/mol	Joback Method
hfus	40.91	kJ/mol	Joback Method
hvap	68.81	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.169		Crippen Method
mcvol	247.670	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	2009.00		NIST Webbook
rinpol	2009.00		NIST Webbook
tb	794.87	K	Joback Method
tc	988.99	K	Joback Method
tf	506.33	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.93	J/mol×K	794.87	Joback Method
cpg	693.95	J/mol×K	827.22	Joback Method
cpg	702.22	J/mol×K	859.58	Joback Method
cpg	709.80	J/mol×K	891.93	Joback Method
cpg	716.78	J/mol×K	924.28	Joback Method
cpg	723.20	J/mol×K	956.64	Joback Method
cpg	729.16	J/mol×K	988.99	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=U405860&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