Fumaric acid, 4-chlorophenyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C15H9ClF8O4/c16-8-1-3-9(4-2-8)28-11(26)6-5-10(25)27-7-13(19,20)15(23,24)14(21,22)12(17)18/h1-6,12H,7H2/b6-5-

InchiKey: CMKCLBYCRXXRGB-AATRIKPKSA-N

Formula: C15H9ClF8O4

SMILES: O=C(C=CC(=O)Oc1ccc(Cl)cc1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 440.67

Physical Properties

Property code	Value	Unit	Source
gf	-1773.75	kJ/mol	Joback Method
hf	-2116.40	kJ/mol	Joback Method
hfus	37.11	kJ/mol	Joback Method
hvap	63.77	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.516		Crippen Method
mcvol	235.430	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	1929.00		NIST Webbook
rinpol	1929.00		NIST Webbook
tb	752.46	K	Joback Method
tc	940.99	K	Joback Method
tf	463.89	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.69	J/mol×K	752.46	Joback Method
cpg	674.81	J/mol×K	783.88	Joback Method
cpg	684.11	J/mol×K	815.30	Joback Method
cpg	692.67	J/mol×K	846.73	Joback Method
cpg	700.54	J/mol×K	878.15	Joback Method
cpg	707.80	J/mol×K	909.57	Joback Method
cpg	714.51	J/mol×K	940.99	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=U405840&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