Fumaric acid, 1-phenylprop-1-yl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C18H16F8O4/c1-2-12(11-6-4-3-5-7-11)30-14(28)9-8-13(27)29-10-16(21,22)18

InchiKey: VDWQZSMOHVNPMM-CMDGGOBGSA-N

Formula: C18H16F8O4

SMILES: CCC(OC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1ccccc1

Mol. weight [g/mol]: 448.30

Physical Properties

Property code	Value	Unit	Source
gf	-1729.37	kJ/mol	Joback Method
hf	-2156.39	kJ/mol	Joback Method
hfus	37.54	kJ/mol	Joback Method
hvap	65.01	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.951		Crippen Method
mcvol	265.460	ml/mol	McGowan Method
pc	1314.65	kPa	Joback Method
rinpol	1925.00		NIST Webbook
rinpol	1925.00		NIST Webbook
tb	778.25	K	Joback Method
tc	964.18	K	Joback Method
tf	440.26	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.93	J/mol×K	778.25	Joback Method
cpg	816.41	J/mol×K	809.24	Joback Method
cpg	827.98	J/mol×K	840.23	Joback Method
cpg	838.72	J/mol×K	871.21	Joback Method
cpg	848.68	J/mol×K	902.20	Joback Method
cpg	857.96	J/mol×K	933.19	Joback Method
cpg	866.61	J/mol×K	964.18	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=U405898&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