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

Inchi: InChI=1S/C17H14F8O4/c18-14(19)16(22,23)17(24,25)15(20,21)10-29-13(27)7-6-12(26)2

InchiKey: MXXYHRPLRPIJBI-VOTSOKGWSA-N

Formula: C17H14F8O4

SMILES: O=C(C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCCc1ccccc1

Mol. weight [g/mol]: 434.28

Physical Properties

Property code	Value	Unit	Source
gf	-1735.35	kJ/mol	Joback Method
hf	-2130.47	kJ/mol	Joback Method
hfus	38.48	kJ/mol	Joback Method
hvap	63.17	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.043		Crippen Method
mcvol	251.370	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
rinpol	1929.00		NIST Webbook
rinpol	1929.00		NIST Webbook
tb	755.81	K	Joback Method
tc	939.19	K	Joback Method
tf	443.99	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.58	J/mol×K	755.81	Joback Method
cpg	760.60	J/mol×K	786.37	Joback Method
cpg	771.74	J/mol×K	816.94	Joback Method
cpg	782.07	J/mol×K	847.50	Joback Method
cpg	791.65	J/mol×K	878.06	Joback Method
cpg	800.55	J/mol×K	908.62	Joback Method
cpg	808.85	J/mol×K	939.19	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=U405677&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