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

Inchi: InChI=1S/C18H16F8O4/c19-15(20)17(23,24)18(25,26)16(21,22)11-30-14(28)9-8-13(27)2

InchiKey: OLOPHWGRMNDZLI-CMDGGOBGSA-N

Formula: C18H16F8O4

SMILES: O=C(C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCCCc1ccccc1

Mol. weight [g/mol]: 448.30

Physical Properties

Property code	Value	Unit	Source
gf	-1726.93	kJ/mol	Joback Method
hf	-2151.11	kJ/mol	Joback Method
hfus	41.07	kJ/mol	Joback Method
hvap	65.40	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.433		Crippen Method
mcvol	265.460	ml/mol	McGowan Method
pc	1307.06	kPa	Joback Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook
tb	778.69	K	Joback Method
tc	963.08	K	Joback Method
tf	455.26	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.36	J/mol×K	778.69	Joback Method
cpg	815.74	J/mol×K	809.42	Joback Method
cpg	827.22	J/mol×K	840.15	Joback Method
cpg	837.89	J/mol×K	870.88	Joback Method
cpg	847.81	J/mol×K	901.62	Joback Method
cpg	857.06	J/mol×K	932.35	Joback Method
cpg	865.71	J/mol×K	963.08	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=U405660&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