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

Inchi: InChI=1S/C17H14F8O6/c1-28-9-4-3-5-10(29-2)13(9)31-12(27)7-6-11(26)30-8-15(20,21)1

InchiKey: MWWNADKBBFZCHQ-VOTSOKGWSA-N

Formula: C17H14F8O6

SMILES: COc1cccc(OC)c1OC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 466.28

Physical Properties

Property code	Value	Unit	Source
gf	-1964.61	kJ/mol	Joback Method
hf	-2417.85	kJ/mol	Joback Method
hfus	40.08	kJ/mol	Joback Method
hvap	69.31	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.880		Crippen Method
mcvol	263.110	ml/mol	McGowan Method
pc	1337.84	kPa	Joback Method
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	810.61	K	Joback Method
tc	999.04	K	Joback Method
tf	513.49	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.28	J/mol×K	810.61	Joback Method
cpg	810.57	J/mol×K	842.01	Joback Method
cpg	820.97	J/mol×K	873.42	Joback Method
cpg	830.52	J/mol×K	904.82	Joback Method
cpg	839.26	J/mol×K	936.23	Joback Method
cpg	847.25	J/mol×K	967.63	Joback Method
cpg	854.52	J/mol×K	999.04	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=U405748&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