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

Inchi: InChI=1S/C17H14F8O4/c1-9-5-10(2)7-11(6-9)29-13(27)4-3-12(26)28-8-15(20,21)17(24,2

InchiKey: FNASLBAIWRVKPF-ONEGZZNKSA-N

Formula: C17H14F8O4

SMILES: Cc1cc(C)cc(OC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1

Mol. weight [g/mol]: 434.28

Physical Properties

Property code	Value	Unit	Source
gf	-1754.61	kJ/mol	Joback Method
hf	-2153.41	kJ/mol	Joback Method
hfus	37.70	kJ/mol	Joback Method
hvap	64.49	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.479		Crippen Method
mcvol	251.370	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	1939.00		NIST Webbook
rinpol	1939.00		NIST Webbook
tb	765.77	K	Joback Method
tc	950.90	K	Joback Method
tf	469.03	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.36	J/mol×K	765.77	Joback Method
cpg	758.18	J/mol×K	796.62	Joback Method
cpg	769.14	J/mol×K	827.48	Joback Method
cpg	779.33	J/mol×K	858.33	Joback Method
cpg	788.79	J/mol×K	889.19	Joback Method
cpg	797.58	J/mol×K	920.04	Joback Method
cpg	805.78	J/mol×K	950.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U405736&Units=SI

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