Fumaric acid, 2,6-dimethoxyphenyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C15H14F4O6/c1-22-9-4-3-5-10(23-2)13(9)25-12(21)7-6-11(20)24-8-15(18,19)1

InchiKey: DELIHFRPFRNKEF-VOTSOKGWSA-N

Formula: C15H14F4O6

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

Mol. weight [g/mol]: 366.26

Physical Properties

Property code	Value	Unit	Source
gf	-1207.89	kJ/mol	Joback Method
hf	-1574.63	kJ/mol	Joback Method
hfus	37.40	kJ/mol	Joback Method
hvap	70.72	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.609		Crippen Method
mcvol	227.850	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	774.23	K	Joback Method
tc	968.34	K	Joback Method
tf	483.75	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.32	J/mol×K	774.23	Joback Method
cpg	667.21	J/mol×K	806.58	Joback Method
cpg	678.22	J/mol×K	838.93	Joback Method
cpg	688.37	J/mol×K	871.29	Joback Method
cpg	697.65	J/mol×K	903.64	Joback Method
cpg	706.09	J/mol×K	935.99	Joback Method
cpg	713.70	J/mol×K	968.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405747&Units=SI
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

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