Fumaric acid, 3,5-dimethylphenyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C15H14F4O4/c1-9-5-10(2)7-11(6-9)23-13(21)4-3-12(20)22-8-15(18,19)14(16)1

InchiKey: UFTUQPATWXOULM-ONEGZZNKSA-N

Formula: C15H14F4O4

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

Mol. weight [g/mol]: 334.26

Physical Properties

Property code	Value	Unit	Source
gf	-997.89	kJ/mol	Joback Method
hf	-1310.19	kJ/mol	Joback Method
hfus	35.03	kJ/mol	Joback Method
hvap	65.90	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.209		Crippen Method
mcvol	216.110	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	1841.00		NIST Webbook
rinpol	1841.00		NIST Webbook
tb	729.39	K	Joback Method
tc	923.77	K	Joback Method
tf	439.29	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.99	J/mol×K	729.39	Joback Method
cpg	615.42	J/mol×K	761.79	Joback Method
cpg	627.02	J/mol×K	794.18	Joback Method
cpg	637.82	J/mol×K	826.58	Joback Method
cpg	647.84	J/mol×K	858.98	Joback Method
cpg	657.14	J/mol×K	891.37	Joback Method
cpg	665.72	J/mol×K	923.77	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=U405735&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