Fumaric acid, ethyl pentafluorophenyl ester

Inchi: InChI=1S/C12H7F5O4/c1-2-20-5(18)3-4-6(19)21-12-10(16)8(14)7(13)9(15)11(12)17/h3-4
InchiKey: QNRCXECFFIGWRM-ONEGZZNKSA-N
Formula: C12H7F5O4
SMILES: CCOC(=O)C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 310.17

Physical Properties

Property code	Value	Unit	Source
gf	-1247.25	kJ/mol	Joback Method
hf	-1464.76	kJ/mol	Joback Method
hfus	40.11	kJ/mol	Joback Method
hvap	62.08	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.407		Crippen Method
mcvol	175.610	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
rinpol	1458.00		NIST Webbook
rinpol	1458.00		NIST Webbook
tb	678.63	K	Joback Method
tc	862.36	K	Joback Method
tf	456.21	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.47	J/mol×K	678.63	Joback Method
cpg	459.09	J/mol×K	709.25	Joback Method
cpg	468.21	J/mol×K	739.87	Joback Method
cpg	476.81	J/mol×K	770.49	Joback Method
cpg	484.89	J/mol×K	801.12	Joback Method
cpg	492.45	J/mol×K	831.74	Joback Method
cpg	499.48	J/mol×K	862.36	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=U348093&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