Fumaric acid, ethyl pentafluorobenzyl ester

Inchi: InChI=1S/C13H9F5O4/c1-2-21-7(19)3-4-8(20)22-5-6-9(14)11(16)13(18)12(17)10(6)15/h3
InchiKey: HIYKWQUZIAKFAY-ONEGZZNKSA-N
Formula: C13H9F5O4
SMILES: CCOC(=O)C=CC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 324.20

Physical Properties

Property code	Value	Unit	Source
gf	-1238.83	kJ/mol	Joback Method
hf	-1485.40	kJ/mol	Joback Method
hfus	42.70	kJ/mol	Joback Method
hvap	64.30	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	2.545		Crippen Method
mcvol	189.700	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook
tb	701.51	K	Joback Method
tc	884.49	K	Joback Method
tf	467.48	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.78	J/mol×K	701.51	Joback Method
cpg	510.07	J/mol×K	732.01	Joback Method
cpg	519.79	J/mol×K	762.50	Joback Method
cpg	528.95	J/mol×K	793.00	Joback Method
cpg	537.54	J/mol×K	823.50	Joback Method
cpg	545.57	J/mol×K	854.00	Joback Method
cpg	553.03	J/mol×K	884.49	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=U405890&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