Fumaric acid, butyl pentafluorophenyl ester

Inchi: InChI=1S/C14H11F5O4/c1-2-3-6-22-7(20)4-5-8(21)23-14-12(18)10(16)9(15)11(17)13(14
InchiKey: YAQIBRZVZVTJQZ-SNAWJCMRSA-N
Formula: C14H11F5O4
SMILES: CCCCOC(=O)C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 338.23

Physical Properties

Property code	Value	Unit	Source
gf	-1230.41	kJ/mol	Joback Method
hf	-1506.04	kJ/mol	Joback Method
hfus	45.29	kJ/mol	Joback Method
hvap	66.53	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.187		Crippen Method
mcvol	203.790	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	1652.00		NIST Webbook
tb	724.39	K	Joback Method
tc	907.10	K	Joback Method
tf	478.75	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.44	J/mol×K	724.39	Joback Method
cpg	562.32	J/mol×K	754.84	Joback Method
cpg	572.60	J/mol×K	785.29	Joback Method
cpg	582.26	J/mol×K	815.74	Joback Method
cpg	591.31	J/mol×K	846.19	Joback Method
cpg	599.75	J/mol×K	876.65	Joback Method
cpg	607.57	J/mol×K	907.10	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=U348096&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