Fumaric acid, isohexyl pentafluorophenyl ester

Inchi: InChI=1S/C16H15F5O4/c1-8(2)4-3-7-24-9(22)5-6-10(23)25-16-14(20)12(18)11(17)13(19

InchiKey: ZUWNWMCKVJOIRL-AATRIKPKSA-N

Formula: C16H15F5O4

SMILES: CC(C)CCCOC(=O)C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 366.28

Physical Properties

Property code	Value	Unit	Source
gf	-1216.01	kJ/mol	Joback Method
hf	-1552.60	kJ/mol	Joback Method
hfus	46.95	kJ/mol	Joback Method
hvap	70.59	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	3.823		Crippen Method
mcvol	231.970	ml/mol	McGowan Method
pc	1512.85	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	769.71	K	Joback Method
tc	955.11	K	Joback Method
tf	486.29	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.99	J/mol×K	769.71	Joback Method
cpg	671.06	J/mol×K	800.61	Joback Method
cpg	682.39	J/mol×K	831.51	Joback Method
cpg	692.99	J/mol×K	862.41	Joback Method
cpg	702.85	J/mol×K	893.31	Joback Method
cpg	712.00	J/mol×K	924.21	Joback Method
cpg	720.43	J/mol×K	955.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348097&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