Fumaric acid, octyl pentafluorophenyl ester

Inchi: InChI=1S/C18H19F5O4/c1-2-3-4-5-6-7-10-26-11(24)8-9-12(25)27-18-16(22)14(20)13(19
InchiKey: GABRCILTWUNFQQ-CMDGGOBGSA-N
Formula: C18H19F5O4
SMILES: CCCCCCCCOC(=O)C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 394.33

Physical Properties

Property code	Value	Unit	Source
gf	-1196.73	kJ/mol	Joback Method
hf	-1588.60	kJ/mol	Joback Method
hfus	55.65	kJ/mol	Joback Method
hvap	75.43	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	4.747		Crippen Method
mcvol	260.150	ml/mol	McGowan Method
pc	1302.35	kPa	Joback Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook
tb	815.91	K	Joback Method
tc	1003.24	K	Joback Method
tf	523.83	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.72	J/mol×K	815.91	Joback Method
cpg	782.63	J/mol×K	847.13	Joback Method
cpg	794.72	J/mol×K	878.35	Joback Method
cpg	805.98	J/mol×K	909.57	Joback Method
cpg	816.43	J/mol×K	940.79	Joback Method
cpg	826.07	J/mol×K	972.02	Joback Method
cpg	834.93	J/mol×K	1003.24	Joback Method

Sources

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=U348100&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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