Fumaric acid, heptyl pentafluorophenyl ester

Inchi: InChI=1S/C17H17F5O4/c1-2-3-4-5-6-9-25-10(23)7-8-11(24)26-17-15(21)13(19)12(18)14
InchiKey: VYWNVCVRWCIBPZ-BQYQJAHWSA-N
Formula: C17H17F5O4
SMILES: CCCCCCCOC(=O)C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 380.31

Physical Properties

Property code	Value	Unit	Source
gf	-1205.15	kJ/mol	Joback Method
hf	-1567.96	kJ/mol	Joback Method
hfus	53.06	kJ/mol	Joback Method
hvap	73.21	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.357		Crippen Method
mcvol	246.060	ml/mol	McGowan Method
pc	1397.50	kPa	Joback Method
rinpol	1958.00		NIST Webbook
tb	793.03	K	Joback Method
tc	978.23	K	Joback Method
tf	512.56	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.57	J/mol×K	793.03	Joback Method
cpg	726.01	J/mol×K	823.90	Joback Method
cpg	737.68	J/mol×K	854.76	Joback Method
cpg	748.59	J/mol×K	885.63	Joback Method
cpg	758.74	J/mol×K	916.50	Joback Method
cpg	768.14	J/mol×K	947.37	Joback Method
cpg	776.80	J/mol×K	978.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348099&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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