Fumaric acid, hexyl pentafluorophenyl ester

Inchi: InChI=1S/C16H15F5O4/c1-2-3-4-5-8-24-9(22)6-7-10(23)25-16-14(20)12(18)11(17)13(19
InchiKey: XHTMSMWXTASNIS-VOTSOKGWSA-N
Formula: C16H15F5O4
SMILES: CCCCCCOC(=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	-1213.57	kJ/mol	Joback Method
hf	-1547.32	kJ/mol	Joback Method
hfus	50.47	kJ/mol	Joback Method
hvap	70.98	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	3.967		Crippen Method
mcvol	231.970	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	1862.00		NIST Webbook
rinpol	1862.00		NIST Webbook
tb	770.15	K	Joback Method
tc	953.91	K	Joback Method
tf	501.29	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.42	J/mol×K	770.15	Joback Method
cpg	670.37	J/mol×K	800.78	Joback Method
cpg	681.61	J/mol×K	831.40	Joback Method
cpg	692.14	J/mol×K	862.03	Joback Method
cpg	701.96	J/mol×K	892.66	Joback Method
cpg	711.08	J/mol×K	923.29	Joback Method
cpg	719.50	J/mol×K	953.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348098&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