Fumaric acid, pentafluorophenyl tetradecyl ester

Inchi: InChI=1S/C24H31F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-32-17(30)14-15-18(31)33-24
InchiKey: LOKAYIIQECNIRC-CCEZHUSRSA-N
Formula: C24H31F5O4
SMILES: CCCCCCCCCCCCCCOC(=O)C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 478.49

Physical Properties

Property code	Value	Unit	Source
gf	-1146.21	kJ/mol	Joback Method
hf	-1712.44	kJ/mol	Joback Method
hfus	71.19	kJ/mol	Joback Method
hvap	88.79	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	7.088		Crippen Method
mcvol	344.690	ml/mol	McGowan Method
pc	892.67	kPa	Joback Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	953.19	K	Joback Method
tc	1171.15	K	Joback Method
tf	591.45	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1123.50	J/mol×K	953.19	Joback Method
cpg	1139.29	J/mol×K	989.52	Joback Method
cpg	1153.72	J/mol×K	1025.84	Joback Method
cpg	1166.81	J/mol×K	1062.17	Joback Method
cpg	1178.61	J/mol×K	1098.50	Joback Method
cpg	1189.14	J/mol×K	1134.83	Joback Method
cpg	1198.44	J/mol×K	1171.15	Joback Method

Sources

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=U348106&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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