Fumaric acid, pentafluorophenyl tridecyl ester

Inchi: InChI=1S/C23H29F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-31-16(29)13-14-17(30)32-23-21
InchiKey: BZEZPFBVHXBGED-BUHFOSPRSA-N
Formula: C23H29F5O4
SMILES: CCCCCCCCCCCCCCOC(=O)C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 464.47

Physical Properties

Property code	Value	Unit	Source
gf	-1154.63	kJ/mol	Joback Method
hf	-1691.80	kJ/mol	Joback Method
hfus	68.60	kJ/mol	Joback Method
hvap	86.56	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	6.698		Crippen Method
mcvol	330.600	ml/mol	McGowan Method
pc	946.16	kPa	Joback Method
rinpol	2522.00		NIST Webbook
rinpol	2522.00		NIST Webbook
tb	930.31	K	Joback Method
tc	1140.68	K	Joback Method
tf	580.18	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.86	J/mol×K	930.31	Joback Method
cpg	1078.14	J/mol×K	965.37	Joback Method
cpg	1092.17	J/mol×K	1000.43	Joback Method
cpg	1104.98	J/mol×K	1035.50	Joback Method
cpg	1116.60	J/mol×K	1070.56	Joback Method
cpg	1127.06	J/mol×K	1105.62	Joback Method
cpg	1136.38	J/mol×K	1140.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348105&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