Fumaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl tridecyl ester

Inchi: InChI=1S/C22H32F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-33-17(31)13-14-18(32)34-16-20
InchiKey: HHMPJJXUNFZZFT-BUHFOSPRSA-N
Formula: C22H32F8O4
SMILES: CCCCCCCCCCCCCOC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 512.47

Physical Properties

Property code	Value	Unit	Source
gf	-1805.66	kJ/mol	Joback Method
hf	-2470.20	kJ/mol	Joback Method
hfus	57.39	kJ/mol	Joback Method
hvap	72.02	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	7.111		Crippen Method
mcvol	345.580	ml/mol	McGowan Method
pc	825.26	kPa	Joback Method
rinpol	2325.00		NIST Webbook
tb	843.53	K	Joback Method
tc	1034.55	K	Joback Method
tf	473.92	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.45	J/mol×K	843.53	Joback Method
cpg	1143.36	J/mol×K	875.37	Joback Method
cpg	1159.24	J/mol×K	907.20	Joback Method
cpg	1174.14	J/mol×K	939.04	Joback Method
cpg	1188.16	J/mol×K	970.87	Joback Method
cpg	1201.39	J/mol×K	1002.71	Joback Method
cpg	1213.90	J/mol×K	1034.55	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=U348789&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