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

Inchi: InChI=1S/C24H38F8O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-35-19(33)15-12-13-16-20(34)36
InchiKey: GGXBTROAOWQASA-UHFFFAOYSA-N
Formula: C24H38F8O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 542.54

Physical Properties

Property code	Value	Unit	Source
gf	-1869.04	kJ/mol	Joback Method
hf	-2628.70	kJ/mol	Joback Method
hfus	62.36	kJ/mol	Joback Method
hvap	76.52	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	8.115		Crippen Method
mcvol	378.060	ml/mol	McGowan Method
pc	720.69	kPa	Joback Method
rinpol	2499.00		NIST Webbook
tb	885.13	K	Joback Method
tc	1093.97	K	Joback Method
tf	501.54	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1275.22	J/mol×K	885.13	Joback Method
cpg	1294.53	J/mol×K	919.94	Joback Method
cpg	1312.51	J/mol×K	954.74	Joback Method
cpg	1329.25	J/mol×K	989.55	Joback Method
cpg	1344.87	J/mol×K	1024.36	Joback Method
cpg	1359.47	J/mol×K	1059.17	Joback Method
cpg	1373.15	J/mol×K	1093.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353738&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

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