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

Inchi: InChI=1S/C23H36F8O4/c1-2-3-4-5-6-7-8-9-10-13-16-34-18(32)14-11-12-15-19(33)35-17

InchiKey: BNJTZUSXJFKODO-UHFFFAOYSA-N

Formula: C23H36F8O4

SMILES: CCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 528.52

Physical Properties

Property code	Value	Unit	Source
gf	-1877.46	kJ/mol	Joback Method
hf	-2608.06	kJ/mol	Joback Method
hfus	59.77	kJ/mol	Joback Method
hvap	74.29	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	7.725		Crippen Method
mcvol	363.970	ml/mol	McGowan Method
pc	759.32	kPa	Joback Method
rinpol	2404.00		NIST Webbook
rinpol	2404.00		NIST Webbook
tb	862.25	K	Joback Method
tc	1061.81	K	Joback Method
tf	490.27	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.57	J/mol×K	862.25	Joback Method
cpg	1232.04	J/mol×K	895.51	Joback Method
cpg	1249.28	J/mol×K	928.77	Joback Method
cpg	1265.38	J/mol×K	962.03	Joback Method
cpg	1280.42	J/mol×K	995.29	Joback Method
cpg	1294.48	J/mol×K	1028.55	Joback Method
cpg	1307.67	J/mol×K	1061.81	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=U353737&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