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

Inchi: InChI=1S/C17H24F8O4/c1-11(2)6-5-9-28-12(26)7-3-4-8-13(27)29-10-15(20,21)17(24,25)

InchiKey: HSJFXNBLURQLBE-UHFFFAOYSA-N

Formula: C17H24F8O4

SMILES: CC(C)CCCOC(=O)CCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 444.36

Physical Properties

Property code	Value	Unit	Source
gf	-1930.42	kJ/mol	Joback Method
hf	-2489.50	kJ/mol	Joback Method
hfus	40.71	kJ/mol	Joback Method
hvap	60.55	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.240		Crippen Method
mcvol	279.430	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
rinpol	1819.00		NIST Webbook
rinpol	1819.00		NIST Webbook
tb	724.53	K	Joback Method
tc	889.95	K	Joback Method
tf	407.65	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.45	J/mol×K	724.53	Joback Method
cpg	874.24	J/mol×K	752.10	Joback Method
cpg	888.18	J/mol×K	779.67	Joback Method
cpg	901.29	J/mol×K	807.24	Joback Method
cpg	913.62	J/mol×K	834.81	Joback Method
cpg	925.21	J/mol×K	862.38	Joback Method
cpg	936.11	J/mol×K	889.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353731&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