Adipic acid, di(2,2,3,3,4,4,5,5-octafluoropentyl) ester

Inchi: InChI=1S/C16H14F16O4/c17-9(18)13(25,26)15(29,30)11(21,22)5-35-7(33)3-1-2-4-8(34)3

InchiKey: NJUJKXGBKIJBHG-UHFFFAOYSA-N

Formula: C16H14F16O4

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

Mol. weight [g/mol]: 574.25

Physical Properties

Property code	Value	Unit	Source
gf	-3488.80	kJ/mol	Joback Method
hf	-4063.99	kJ/mol	Joback Method
hfus	40.52	kJ/mol	Joback Method
hvap	47.90	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.975		Crippen Method
mcvol	279.500	ml/mol	McGowan Method
pc	945.58	kPa	Joback Method
rinpol	1605.00		NIST Webbook
tb	686.12	K	Joback Method
tc	840.08	K	Joback Method
tf	408.36	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.57	J/mol×K	686.12	Joback Method
cpg	886.32	J/mol×K	711.78	Joback Method
cpg	898.19	J/mol×K	737.44	Joback Method
cpg	909.25	J/mol×K	763.10	Joback Method
cpg	919.54	J/mol×K	788.76	Joback Method
cpg	929.13	J/mol×K	814.42	Joback Method
cpg	938.07	J/mol×K	840.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353745&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