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

Inchi: InChI=1S/C16H22F8O4/c1-2-3-6-9-27-11(25)7-4-5-8-12(26)28-10-14(19,20)16(23,24)15

InchiKey: XKVYIVSCEXZTFA-UHFFFAOYSA-N

Formula: C16H22F8O4

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

Mol. weight [g/mol]: 430.33

Physical Properties

Property code	Value	Unit	Source
gf	-1936.40	kJ/mol	Joback Method
hf	-2463.58	kJ/mol	Joback Method
hfus	41.64	kJ/mol	Joback Method
hvap	58.71	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.994		Crippen Method
mcvol	265.340	ml/mol	McGowan Method
pc	1143.66	kPa	Joback Method
rinpol	1764.00		NIST Webbook
rinpol	1764.00		NIST Webbook
tb	702.09	K	Joback Method
tc	863.81	K	Joback Method
tf	411.38	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.93	J/mol×K	702.09	Joback Method
cpg	817.15	J/mol×K	729.04	Joback Method
cpg	830.55	J/mol×K	756.00	Joback Method
cpg	843.19	J/mol×K	782.95	Joback Method
cpg	855.09	J/mol×K	809.90	Joback Method
cpg	866.30	J/mol×K	836.85	Joback Method
cpg	876.84	J/mol×K	863.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353730&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