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

Inchi: InChI=1S/C27H44F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-20-38-22(36)18-15-16-19

InchiKey: LEYYNNHCNJOMHL-UHFFFAOYSA-N

Formula: C27H44F8O4

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

Mol. weight [g/mol]: 584.62

Physical Properties

Property code	Value	Unit	Source
gf	-1843.78	kJ/mol	Joback Method
hf	-2690.62	kJ/mol	Joback Method
hfus	70.13	kJ/mol	Joback Method
hvap	83.20	kJ/mol	Joback Method
log10ws	-10.11		Crippen Method
logp	9.286		Crippen Method
mcvol	420.330	ml/mol	McGowan Method
pc	620.96	kPa	Joback Method
rinpol	2778.00		NIST Webbook
rinpol	2778.00		NIST Webbook
tb	953.77	K	Joback Method
tc	1198.31	K	Joback Method
tf	535.35	K	Joback Method
vc	1.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1463.63	J/mol×K	953.77	Joback Method
cpg	1485.97	J/mol×K	994.53	Joback Method
cpg	1506.59	J/mol×K	1035.28	Joback Method
cpg	1525.67	J/mol×K	1076.04	Joback Method
cpg	1543.41	J/mol×K	1116.80	Joback Method
cpg	1559.97	J/mol×K	1157.56	Joback Method
cpg	1575.53	J/mol×K	1198.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353741&Units=SI

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