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

Inchi: InChI=1S/C29H48F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-40-24(38)20-17
InchiKey: RJXNBVTVZREHGI-UHFFFAOYSA-N
Formula: C29H48F8O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 612.68

Physical Properties

Property code	Value	Unit	Source
gf	-1826.94	kJ/mol	Joback Method
hf	-2731.90	kJ/mol	Joback Method
hfus	75.31	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-10.94		Crippen Method
logp	10.066		Crippen Method
mcvol	448.510	ml/mol	McGowan Method
pc	565.55	kPa	Joback Method
rinpol	2979.00		NIST Webbook
rinpol	2979.00		NIST Webbook
tb	999.53	K	Joback Method
tc	1275.61	K	Joback Method
tf	557.89	K	Joback Method
vc	1.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1591.75	J/mol×K	999.53	Joback Method
cpg	1616.63	J/mol×K	1045.54	Joback Method
cpg	1639.47	J/mol×K	1091.56	Joback Method
cpg	1660.54	J/mol×K	1137.57	Joback Method
cpg	1680.12	J/mol×K	1183.58	Joback Method
cpg	1698.48	J/mol×K	1229.59	Joback Method
cpg	1715.88	J/mol×K	1275.61	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=U353743&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