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

Inchi: InChI=1S/C19H28F8O4/c1-2-3-4-5-6-9-12-30-14(28)10-7-8-11-15(29)31-13-17(22,23)19

InchiKey: DCFXMIGVWPCTGF-UHFFFAOYSA-N

Formula: C19H28F8O4

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

Mol. weight [g/mol]: 472.41

Physical Properties

Property code	Value	Unit	Source
gf	-1911.14	kJ/mol	Joback Method
hf	-2525.50	kJ/mol	Joback Method
hfus	49.41	kJ/mol	Joback Method
hvap	65.39	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.165		Crippen Method
mcvol	307.610	ml/mol	McGowan Method
pc	949.67	kPa	Joback Method
rinpol	2036.00		NIST Webbook
rinpol	2036.00		NIST Webbook
tb	770.73	K	Joback Method
tc	943.64	K	Joback Method
tf	445.19	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	973.89	J/mol×K	770.73	Joback Method
cpg	989.67	J/mol×K	799.55	Joback Method
cpg	1004.51	J/mol×K	828.37	Joback Method
cpg	1018.45	J/mol×K	857.19	Joback Method
cpg	1031.56	J/mol×K	886.00	Joback Method
cpg	1043.87	J/mol×K	914.82	Joback Method
cpg	1055.44	J/mol×K	943.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353734&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