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

Inchi: InChI=1S/C28H46F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-39-23(37)19-16-17

InchiKey: ZAVITWUAPBXDAE-UHFFFAOYSA-N

Formula: C28H46F8O4

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

Mol. weight [g/mol]: 598.65

Physical Properties

Property code	Value	Unit	Source
gf	-1835.36	kJ/mol	Joback Method
hf	-2711.26	kJ/mol	Joback Method
hfus	72.72	kJ/mol	Joback Method
hvap	85.42	kJ/mol	Joback Method
log10ws	-10.52		Crippen Method
logp	9.676		Crippen Method
mcvol	434.420	ml/mol	McGowan Method
pc	592.28	kPa	Joback Method
rinpol	2871.00		NIST Webbook
rinpol	2871.00		NIST Webbook
tb	976.65	K	Joback Method
tc	1236.10	K	Joback Method
tf	546.62	K	Joback Method
vc	1.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1527.46	J/mol×K	976.65	Joback Method
cpg	1551.01	J/mol×K	1019.89	Joback Method
cpg	1572.68	J/mol×K	1063.13	Joback Method
cpg	1592.71	J/mol×K	1106.37	Joback Method
cpg	1611.31	J/mol×K	1149.62	Joback Method
cpg	1628.71	J/mol×K	1192.86	Joback Method
cpg	1645.11	J/mol×K	1236.10	Joback Method

Sources

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=U353742&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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