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

Inchi: InChI=1S/C33H56F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-20-23-26-44-28(42)24-21

InchiKey: VKLCKQUBDVRKLR-UHFFFAOYSA-N

Formula: C33H56F8O4

SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 668.78

Physical Properties

Property code	Value	Unit	Source
gf	-1793.26	kJ/mol	Joback Method
hf	-2814.46	kJ/mol	Joback Method
hfus	85.68	kJ/mol	Joback Method
hvap	96.55	kJ/mol	Joback Method
log10ws	-12.62		Crippen Method
logp	11.626		Crippen Method
mcvol	504.870	ml/mol	McGowan Method
pc	474.86	kPa	Joback Method
rinpol	3392.00		NIST Webbook
tb	1091.05	K	Joback Method
tc	1454.16	K	Joback Method
tf	602.97	K	Joback Method
vc	2.037	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1852.98	J/mol×K	1091.05	Joback Method
cpg	1884.73	J/mol×K	1151.57	Joback Method
cpg	1913.65	J/mol×K	1212.09	Joback Method
cpg	1940.42	J/mol×K	1272.61	Joback Method
cpg	1965.72	J/mol×K	1333.13	Joback Method
cpg	1990.24	J/mol×K	1393.64	Joback Method
cpg	2014.66	J/mol×K	1454.16	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=U355750&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