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

Inchi: InChI=1S/C30H50F8O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-20-23-41-25(39)21-18-15-12-13

InchiKey: UJWGLBYDPPCTOY-UHFFFAOYSA-N

Formula: C30H50F8O4

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

Mol. weight [g/mol]: 626.70

Physical Properties

Property code	Value	Unit	Source
gf	-1818.52	kJ/mol	Joback Method
hf	-2752.54	kJ/mol	Joback Method
hfus	77.91	kJ/mol	Joback Method
hvap	89.87	kJ/mol	Joback Method
log10ws	-11.36		Crippen Method
logp	10.456		Crippen Method
mcvol	462.600	ml/mol	McGowan Method
pc	540.58	kPa	Joback Method
rinpol	3101.00		NIST Webbook
rinpol	3101.00		NIST Webbook
tb	1022.41	K	Joback Method
tc	1316.99	K	Joback Method
tf	569.16	K	Joback Method
vc	1.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1656.46	J/mol×K	1022.41	Joback Method
cpg	1682.82	J/mol×K	1071.51	Joback Method
cpg	1706.94	J/mol×K	1120.60	Joback Method
cpg	1729.18	J/mol×K	1169.70	Joback Method
cpg	1749.88	J/mol×K	1218.79	Joback Method
cpg	1769.36	J/mol×K	1267.89	Joback Method
cpg	1787.98	J/mol×K	1316.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355747&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