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

Inchi: InChI=1S/C31H52F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-18-21-24-42-26(40)22-19-16-13

InchiKey: CYMGUSZRRNNDQG-UHFFFAOYSA-N

Formula: C31H52F8O4

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

Mol. weight [g/mol]: 640.73

Physical Properties

Property code	Value	Unit	Source
gf	-1810.10	kJ/mol	Joback Method
hf	-2773.18	kJ/mol	Joback Method
hfus	80.50	kJ/mol	Joback Method
hvap	92.10	kJ/mol	Joback Method
log10ws	-11.78		Crippen Method
logp	10.846		Crippen Method
mcvol	476.690	ml/mol	McGowan Method
pc	517.23	kPa	Joback Method
rinpol	3198.00		NIST Webbook
tb	1045.29	K	Joback Method
tc	1360.41	K	Joback Method
tf	580.43	K	Joback Method
vc	1.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1721.59	J/mol×K	1045.29	Joback Method
cpg	1749.56	J/mol×K	1097.81	Joback Method
cpg	1775.11	J/mol×K	1150.33	Joback Method
cpg	1798.67	J/mol×K	1202.85	Joback Method
cpg	1820.65	J/mol×K	1255.37	Joback Method
cpg	1841.49	J/mol×K	1307.89	Joback Method
cpg	1861.61	J/mol×K	1360.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355748&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