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

Inchi: InChI=1S/C25H40F8O4/c1-2-3-4-5-6-9-12-15-18-36-20(34)16-13-10-7-8-11-14-17-21(35

InchiKey: HHXUFYWLDZOBAM-UHFFFAOYSA-N

Formula: C25H40F8O4

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

Mol. weight [g/mol]: 556.57

Physical Properties

Property code	Value	Unit	Source
gf	-1860.62	kJ/mol	Joback Method
hf	-2649.34	kJ/mol	Joback Method
hfus	64.95	kJ/mol	Joback Method
hvap	78.74	kJ/mol	Joback Method
log10ws	-9.27		Crippen Method
logp	8.505		Crippen Method
mcvol	392.150	ml/mol	McGowan Method
pc	684.93	kPa	Joback Method
rinpol	2616.00		NIST Webbook
rinpol	2616.00		NIST Webbook
tb	908.01	K	Joback Method
tc	1127.37	K	Joback Method
tf	512.81	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1337.48	J/mol×K	908.01	Joback Method
cpg	1357.70	J/mol×K	944.57	Joback Method
cpg	1376.48	J/mol×K	981.13	Joback Method
cpg	1393.94	J/mol×K	1017.69	Joback Method
cpg	1410.20	J/mol×K	1054.25	Joback Method
cpg	1425.38	J/mol×K	1090.81	Joback Method
cpg	1439.60	J/mol×K	1127.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355742&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