Succinic acid, 2,2,3,3-tetrafluoropropyl tetradec-3-en-1-yl ester

Inchi: InChI=1S/C21H34F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-28-18(26)14-15-19(27)29-17

InchiKey: AVKPCYQYQDWABM-VAWYXSNFSA-N

Formula: C21H34F4O4

SMILES: CCCCCCCCCCC=CCCOC(=O)CCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 426.49

Physical Properties

Property code	Value	Unit	Source
gf	-1040.52	kJ/mol	Joback Method
hf	-1647.62	kJ/mol	Joback Method
hfus	57.30	kJ/mol	Joback Method
hvap	75.66	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	6.231		Crippen Method
mcvol	324.410	ml/mol	McGowan Method
pc	950.84	kPa	Joback Method
rinpol	2351.00		NIST Webbook
tb	830.03	K	Joback Method
tc	1016.19	K	Joback Method
tf	455.45	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.11	J/mol×K	830.03	Joback Method
cpg	1052.32	J/mol×K	861.06	Joback Method
cpg	1068.51	J/mol×K	892.08	Joback Method
cpg	1083.72	J/mol×K	923.11	Joback Method
cpg	1098.00	J/mol×K	954.14	Joback Method
cpg	1111.38	J/mol×K	985.16	Joback Method
cpg	1123.93	J/mol×K	1016.19	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391051&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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