Succinic acid, 2,2,3,3-tetrafluoropropyl hept-1,6-dien-4-yl ester

Inchi: InChI=1S/C14H18F4O4/c1-3-5-10(6-4-2)22-12(20)8-7-11(19)21-9-14(17,18)13(15)16/h3-

InchiKey: XJHNOORFJYSALI-UHFFFAOYSA-N

Formula: C14H18F4O4

SMILES: C=CCC(CC=C)OC(=O)CCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 326.28

Physical Properties

Property code	Value	Unit	Source
gf	-1006.44	kJ/mol	Joback Method
hf	-1374.78	kJ/mol	Joback Method
hfus	32.89	kJ/mol	Joback Method
hvap	58.39	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.274		Crippen Method
mcvol	221.480	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	1540.00		NIST Webbook
rinpol	1540.00		NIST Webbook
tb	658.63	K	Joback Method
tc	827.99	K	Joback Method
tf	363.12	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.51	J/mol×K	658.63	Joback Method
cpg	624.90	J/mol×K	686.86	Joback Method
cpg	637.58	J/mol×K	715.08	Joback Method
cpg	649.57	J/mol×K	743.31	Joback Method
cpg	660.89	J/mol×K	771.53	Joback Method
cpg	671.56	J/mol×K	799.76	Joback Method
cpg	681.60	J/mol×K	827.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391326&Units=SI

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