Succinic acid, 2,2,3,3-tetrafluoropropyl pentafluorophenyl ester

Inchi: InChI=1S/C13H7F9O4/c14-6-7(15)9(17)11(10(18)8(6)16)26-5(24)2-1-4(23)25-3-13(21,22
InchiKey: DFXWRIJVBQJWTC-UHFFFAOYSA-N
Formula: C13H7F9O4
SMILES: O=C(CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 398.18

Physical Properties

Property code	Value	Unit	Source
gf	-2097.89	kJ/mol	Joback Method
hf	-2401.09	kJ/mol	Joback Method
hfus	43.88	kJ/mol	Joback Method
hvap	59.39	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	3.511		Crippen Method
mcvol	201.080	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
tb	690.76	K	Joback Method
tc	857.80	K	Joback Method
tf	462.34	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.63	J/mol×K	690.76	Joback Method
cpg	568.42	J/mol×K	718.60	Joback Method
cpg	577.66	J/mol×K	746.44	Joback Method
cpg	586.34	J/mol×K	774.28	Joback Method
cpg	594.47	J/mol×K	802.12	Joback Method
cpg	602.06	J/mol×K	829.96	Joback Method
cpg	609.12	J/mol×K	857.80	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=U390345&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