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

Inchi: InChI=1S/C12H18F4O4/c1-11(2,3)6-19-8(17)4-5-9(18)20-7-12(15,16)10(13)14/h10H,4-7

InchiKey: HNPBHJQTRCOOMW-UHFFFAOYSA-N

Formula: C12H18F4O4

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

Mol. weight [g/mol]: 302.26

Physical Properties

Property code	Value	Unit	Source
gf	-1193.68	kJ/mol	Joback Method
hf	-1587.83	kJ/mol	Joback Method
hfus	26.38	kJ/mol	Joback Method
hvap	54.37	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.799		Crippen Method
mcvol	201.900	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	1359.00		NIST Webbook
rinpol	1359.00		NIST Webbook
tb	616.72	K	Joback Method
tc	786.51	K	Joback Method
tf	361.52	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.66	J/mol×K	616.72	Joback Method
cpg	568.30	J/mol×K	645.02	Joback Method
cpg	581.21	J/mol×K	673.32	Joback Method
cpg	593.42	J/mol×K	701.62	Joback Method
cpg	604.96	J/mol×K	729.92	Joback Method
cpg	615.83	J/mol×K	758.22	Joback Method
cpg	626.07	J/mol×K	786.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389575&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

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