Succinic acid, di(2,2,3,4,4,4-hexafluorobutyl) ester

Inchi: InChI=1S/C12H10F12O4/c13-7(11(19,20)21)9(15,16)3-27-5(25)1-2-6(26)28-4-10(17,18)8

InchiKey: ZVNBCDAFCXAIGY-UHFFFAOYSA-N

Formula: C12H10F12O4

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

Mol. weight [g/mol]: 446.19

Physical Properties

Property code	Value	Unit	Source
gf	-2748.92	kJ/mol	Joback Method
hf	-3179.49	kJ/mol	Joback Method
hfus	32.67	kJ/mol	Joback Method
hvap	44.85	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.924		Crippen Method
mcvol	216.060	ml/mol	McGowan Method
pc	1345.70	kPa	Joback Method
rinpol	1258.00		NIST Webbook
rinpol	1258.00		NIST Webbook
tb	603.98	K	Joback Method
tc	749.46	K	Joback Method
tf	356.08	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.95	J/mol×K	603.98	Joback Method
cpg	637.42	J/mol×K	628.23	Joback Method
cpg	648.19	J/mol×K	652.47	Joback Method
cpg	658.31	J/mol×K	676.72	Joback Method
cpg	667.80	J/mol×K	700.97	Joback Method
cpg	676.69	J/mol×K	725.21	Joback Method
cpg	685.02	J/mol×K	749.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390817&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