Succinic acid, 1,1,1-trifluoroprop-2-yl neopentyl ester

Inchi: InChI=1S/C12H19F3O4/c1-8(12(13,14)15)19-10(17)6-5-9(16)18-7-11(2,3)4/h8H,5-7H2,1

InchiKey: SBEHBMOURMEUHM-UHFFFAOYSA-N

Formula: C12H19F3O4

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

Mol. weight [g/mol]: 284.27

Physical Properties

Property code	Value	Unit	Source
gf	-998.87	kJ/mol	Joback Method
hf	-1391.72	kJ/mol	Joback Method
hfus	23.30	kJ/mol	Joback Method
hvap	55.19	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.850		Crippen Method
mcvol	200.130	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	1272.00		NIST Webbook
rinpol	1272.00		NIST Webbook
tb	617.45	K	Joback Method
tc	793.52	K	Joback Method
tf	360.93	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.59	J/mol×K	617.45	Joback Method
cpg	560.77	J/mol×K	646.79	Joback Method
cpg	574.17	J/mol×K	676.14	Joback Method
cpg	586.83	J/mol×K	705.48	Joback Method
cpg	598.78	J/mol×K	734.83	Joback Method
cpg	610.02	J/mol×K	764.17	Joback Method
cpg	620.59	J/mol×K	793.52	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=U389574&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