Succinic acid, 2,2,3,3-tetrafluoropropyl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C19H28F4O4/c1-2-3-4-5-6-7-8-9-10-11-14-26-16(24)12-13-17(25)27-15-19(22
InchiKey: OTBVDCAYSZPAKL-UHFFFAOYSA-N
Formula: C19H28F4O4
SMILES: CCC#CCCCCCCCCOC(=O)CCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 396.42

Physical Properties

Property code	Value	Unit	Source
gf	-934.78	kJ/mol	Joback Method
hf	-1451.26	kJ/mol	Joback Method
hfus	55.04	kJ/mol	Joback Method
hvap	73.40	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.897		Crippen Method
mcvol	291.930	ml/mol	McGowan Method
pc	1154.57	kPa	Joback Method
tb	789.11	K	Joback Method
tc	970.44	K	Joback Method
tf	544.09	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.39	J/mol×K	789.11	Joback Method
cpg	908.12	J/mol×K	819.33	Joback Method
cpg	922.92	J/mol×K	849.55	Joback Method
cpg	936.82	J/mol×K	879.78	Joback Method
cpg	949.85	J/mol×K	910.00	Joback Method
cpg	962.04	J/mol×K	940.22	Joback Method
cpg	973.41	J/mol×K	970.44	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=U390992&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume