Succinic acid, tridec-2-yn-1-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C20H29F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-28-17(26)13-14-18(27)29-16-19

InchiKey: NUZZBVMQLARBJQ-UHFFFAOYSA-N

Formula: C20H29F5O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 428.43

Physical Properties

Property code	Value	Unit	Source
gf	-1115.89	kJ/mol	Joback Method
hf	-1671.48	kJ/mol	Joback Method
hfus	56.82	kJ/mol	Joback Method
hvap	73.90	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.585		Crippen Method
mcvol	307.790	ml/mol	McGowan Method
pc	1058.95	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
tb	808.47	K	Joback Method
tc	991.76	K	Joback Method
tf	573.37	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	959.27	J/mol×K	808.47	Joback Method
cpg	975.03	J/mol×K	839.02	Joback Method
cpg	989.83	J/mol×K	869.57	Joback Method
cpg	1003.73	J/mol×K	900.11	Joback Method
cpg	1016.76	J/mol×K	930.66	Joback Method
cpg	1028.97	J/mol×K	961.21	Joback Method
cpg	1040.40	J/mol×K	991.76	Joback Method

Sources

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=U390877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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