Succinic acid, 2,2,3,3-tetrafluoropropyl adamant-2-yl ester

Inchi: InChI=1S/C17H22F4O4/c18-16(19)17(20,21)8-24-13(22)1-2-14(23)25-15-11-4-9-3-10(6-

InchiKey: AQYZKYDQOJJBCZ-UHFFFAOYSA-N

Formula: C17H22F4O4

SMILES: O=C(CCC(=O)OC1C2CC3CC(C2)CC1C3)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 366.35

Physical Properties

Property code	Value	Unit	Source
gf	-999.69	kJ/mol	Joback Method
hf	-1510.72	kJ/mol	Joback Method
hfus	41.19	kJ/mol	Joback Method
hvap	66.09	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.578		Crippen Method
mcvol	239.770	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2084.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	749.50	K	Joback Method
tc	939.41	K	Joback Method
tf	457.27	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.36	J/mol×K	749.50	Joback Method
cpg	804.22	J/mol×K	781.15	Joback Method
cpg	820.04	J/mol×K	812.80	Joback Method
cpg	834.88	J/mol×K	844.45	Joback Method
cpg	848.82	J/mol×K	876.10	Joback Method
cpg	861.92	J/mol×K	907.75	Joback Method
cpg	874.26	J/mol×K	939.41	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=U391338&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