Succinic acid, (adamant-1-yl)methyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C18H24F4O4/c19-16(20)18(21,22)10-26-15(24)2-1-14(23)25-9-17-6-11-3-12(7

InchiKey: PJDDEKSQYYFRBL-UHFFFAOYSA-N

Formula: C18H24F4O4

SMILES: O=C(CCC(=O)OCC(F)(F)C(F)F)OCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 380.37

Physical Properties

Property code	Value	Unit	Source
gf	-989.05	kJ/mol	Joback Method
hf	-1495.78	kJ/mol	Joback Method
hfus	36.41	kJ/mol	Joback Method
hvap	67.47	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.970		Crippen Method
mcvol	253.860	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	2182.00		NIST Webbook
rinpol	2182.00		NIST Webbook
tb	777.29	K	Joback Method
tc	971.41	K	Joback Method
tf	496.68	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.37	J/mol×K	777.29	Joback Method
cpg	854.71	J/mol×K	809.64	Joback Method
cpg	871.40	J/mol×K	842.00	Joback Method
cpg	887.58	J/mol×K	874.35	Joback Method
cpg	903.39	J/mol×K	906.70	Joback Method
cpg	918.99	J/mol×K	939.06	Joback Method
cpg	934.51	J/mol×K	971.41	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=U391352&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