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

Inchi: InChI=1S/C19H26F4O4/c20-17(21)19(22,23)11-27-16(25)2-1-15(24)26-4-3-18-8-12-5-13

InchiKey: YHLBXLQNCBMHAD-UHFFFAOYSA-N

Formula: C19H26F4O4

SMILES: O=C(CCC(=O)OCC(F)(F)C(F)F)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 394.40

Physical Properties

Property code	Value	Unit	Source
gf	-980.63	kJ/mol	Joback Method
hf	-1516.42	kJ/mol	Joback Method
hfus	39.00	kJ/mol	Joback Method
hvap	69.70	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.360		Crippen Method
mcvol	267.950	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
rinpol	2325.00		NIST Webbook
rinpol	2325.00		NIST Webbook
tb	800.17	K	Joback Method
tc	994.39	K	Joback Method
tf	507.95	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.08	J/mol×K	800.17	Joback Method
cpg	913.92	J/mol×K	832.54	Joback Method
cpg	931.16	J/mol×K	864.91	Joback Method
cpg	947.95	J/mol×K	897.28	Joback Method
cpg	964.42	J/mol×K	929.65	Joback Method
cpg	980.74	J/mol×K	962.02	Joback Method
cpg	997.03	J/mol×K	994.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391361&Units=SI
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

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