Succinic acid, 1,1,1-trifluoroprop-2-yl adamant-2-yl ester

Inchi: InChI=1S/C17H23F3O4/c1-9(17(18,19)20)23-14(21)2-3-15(22)24-16-12-5-10-4-11(7-12)6-13(16)8-10/h9-13,16H,2-8H2,1H3

InchiKey: LRMRJPJOMJVPLJ-UHFFFAOYSA-N

Formula: C17H23F3O4

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

Mol. weight [g/mol]: 348.36

Physical Properties

Property code	Value	Unit	Source
gf	-804.88	kJ/mol	Joback Method
hf	-1314.61	kJ/mol	Joback Method
hfus	38.11	kJ/mol	Joback Method
hvap	66.91	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.628		Crippen Method
mcvol	238.000	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
tb	750.23	K	Joback Method
tc	945.81	K	Joback Method
tf	456.68	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.70	J/mol×K	750.23	Joback Method
cpg	797.14	J/mol×K	782.83	Joback Method
cpg	813.48	J/mol×K	815.42	Joback Method
cpg	828.80	J/mol×K	848.02	Joback Method
cpg	843.17	J/mol×K	880.62	Joback Method
cpg	856.67	J/mol×K	913.21	Joback Method
cpg	869.37	J/mol×K	945.81	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=U391337&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