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

Inchi: InChI=1S/C11H17F3O5/c1-3-17-6-7-18-9(15)4-5-10(16)19-8(2)11(12,13)14/h8H,3-7H2,1

InchiKey: JLUWHQYFJWEJHN-UHFFFAOYSA-N

Formula: C11H17F3O5

SMILES: CCOCCOC(=O)CCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 286.24

Physical Properties

Property code	Value	Unit	Source
gf	-1115.13	kJ/mol	Joback Method
hf	-1494.55	kJ/mol	Joback Method
hfus	29.31	kJ/mol	Joback Method
hvap	56.67	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.840		Crippen Method
mcvol	191.910	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	1374.00		NIST Webbook
rinpol	1374.00		NIST Webbook
tb	620.22	K	Joback Method
tc	789.61	K	Joback Method
tf	369.47	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.32	J/mol×K	620.22	Joback Method
cpg	532.24	J/mol×K	648.45	Joback Method
cpg	544.55	J/mol×K	676.68	Joback Method
cpg	556.26	J/mol×K	704.91	Joback Method
cpg	567.38	J/mol×K	733.15	Joback Method
cpg	577.90	J/mol×K	761.38	Joback Method
cpg	587.83	J/mol×K	789.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390659&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