Succinic acid, hept-2-yl 2-fluoroethyl ester

Inchi: InChI=1S/C13H23FO4/c1-3-4-5-6-11(2)18-13(16)8-7-12(15)17-10-9-14/h11H,3-10H2,1-2
InchiKey: ABIINXBGFGNUNB-UHFFFAOYSA-N
Formula: C13H23FO4
SMILES: CCCCCC(C)OC(=O)CCC(=O)OCCF
Mol. weight [g/mol]: 262.32

Physical Properties

Property code	Value	Unit	Source
gf	-606.51	kJ/mol	Joback Method
hf	-1002.64	kJ/mol	Joback Method
hfus	34.56	kJ/mol	Joback Method
hvap	61.64	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.791		Crippen Method
mcvol	210.680	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	1684.00		NIST Webbook
rinpol	1684.00		NIST Webbook
tb	648.25	K	Joback Method
tc	821.35	K	Joback Method
tf	366.18	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.79	J/mol×K	648.25	Joback Method
cpg	591.62	J/mol×K	677.10	Joback Method
cpg	605.77	J/mol×K	705.95	Joback Method
cpg	619.26	J/mol×K	734.80	Joback Method
cpg	632.09	J/mol×K	763.65	Joback Method
cpg	644.26	J/mol×K	792.50	Joback Method
cpg	655.77	J/mol×K	821.35	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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