Succinic acid, cyclohexylmethyl 2-fluoroethyl ester

Inchi: InChI=1S/C13H21FO4/c14-8-9-17-12(15)6-7-13(16)18-10-11-4-2-1-3-5-11/h11H,1-10H2

InchiKey: OMSUINKBDSPRTM-UHFFFAOYSA-N

Formula: C13H21FO4

SMILES: O=C(CCC(=O)OCC1CCCCC1)OCCF

Mol. weight [g/mol]: 260.30

Physical Properties

Property code	Value	Unit	Source
gf	-579.62	kJ/mol	Joback Method
hf	-943.04	kJ/mol	Joback Method
hfus	29.92	kJ/mol	Joback Method
hvap	62.46	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.403		Crippen Method
mcvol	199.820	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook
tb	668.24	K	Joback Method
tc	862.53	K	Joback Method
tf	388.56	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.11	J/mol×K	668.24	Joback Method
cpg	585.95	J/mol×K	700.62	Joback Method
cpg	601.84	J/mol×K	733.00	Joback Method
cpg	616.78	J/mol×K	765.39	Joback Method
cpg	630.77	J/mol×K	797.77	Joback Method
cpg	643.83	J/mol×K	830.15	Joback Method
cpg	655.95	J/mol×K	862.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390881&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

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