Succinic acid, ethyl (5-ethyl-1,3-dioxan-5-yl)methyl ester

Inchi: InChI=1S/C13H22O6/c1-3-13(7-16-10-17-8-13)9-19-12(15)6-5-11(14)18-4-2/h3-10H2,1-2

InchiKey: DXLIEZBBXFWGII-UHFFFAOYSA-N

Formula: C13H22O6

SMILES: CCOC(=O)CCC(=O)OCC1(CC)COCOC1

Mol. weight [g/mol]: 274.31

Physical Properties

Property code	Value	Unit	Source
gf	-562.54	kJ/mol	Joback Method
hf	-995.69	kJ/mol	Joback Method
hfus	36.49	kJ/mol	Joback Method
hvap	71.14	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.274		Crippen Method
mcvol	209.790	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
rinpol	1880.00		NIST Webbook
rinpol	1880.00		NIST Webbook
tb	723.11	K	Joback Method
tc	929.17	K	Joback Method
tf	465.01	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.48	J/mol×K	723.11	Joback Method
cpg	638.71	J/mol×K	757.45	Joback Method
cpg	654.20	J/mol×K	791.80	Joback Method
cpg	669.02	J/mol×K	826.14	Joback Method
cpg	683.25	J/mol×K	860.48	Joback Method
cpg	696.96	J/mol×K	894.83	Joback Method
cpg	710.22	J/mol×K	929.17	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382202&Units=SI

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