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

Inchi: InChI=1S/C18H30O8/c1-3-17(7-21-13-22-8-17)11-25-15(19)5-6-16(20)26-12-18(4-2)9-23

InchiKey: JTVMBXZGZVQILB-UHFFFAOYSA-N

Formula: C18H30O8

SMILES: CCC1(COC(=O)CCC(=O)OCC2(CC)COCOC2)COCOC1

Mol. weight [g/mol]: 374.43

Physical Properties

Property code	Value	Unit	Source
gf	-673.72	kJ/mol	Joback Method
hf	-1293.33	kJ/mol	Joback Method
hfus	50.94	kJ/mol	Joback Method
hvap	90.57	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.654		Crippen Method
mcvol	281.120	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook
tb	911.20	K	Joback Method
tc	1136.86	K	Joback Method
tf	605.78	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.77	J/mol×K	911.20	Joback Method
cpg	996.41	J/mol×K	948.81	Joback Method
cpg	1018.04	J/mol×K	986.42	Joback Method
cpg	1039.89	J/mol×K	1024.03	Joback Method
cpg	1062.14	J/mol×K	1061.64	Joback Method
cpg	1085.02	J/mol×K	1099.25	Joback Method
cpg	1108.74	J/mol×K	1136.86	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=U382215&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