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

Inchi: InChI=1S/C14H24O6/c1-3-7-19-12(15)5-6-13(16)20-10-14(4-2)8-17-11-18-9-14/h3-11H2

InchiKey: IOUWOUUOJBEKNI-UHFFFAOYSA-N

Formula: C14H24O6

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

Mol. weight [g/mol]: 288.34

Physical Properties

Property code	Value	Unit	Source
gf	-554.12	kJ/mol	Joback Method
hf	-1016.33	kJ/mol	Joback Method
hfus	39.09	kJ/mol	Joback Method
hvap	73.37	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.664		Crippen Method
mcvol	223.880	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	1983.00		NIST Webbook
rinpol	1983.00		NIST Webbook
tb	745.99	K	Joback Method
tc	949.94	K	Joback Method
tf	476.28	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.01	J/mol×K	745.99	Joback Method
cpg	694.69	J/mol×K	779.98	Joback Method
cpg	710.63	J/mol×K	813.97	Joback Method
cpg	725.91	J/mol×K	847.97	Joback Method
cpg	740.60	J/mol×K	881.96	Joback Method
cpg	754.77	J/mol×K	915.95	Joback Method
cpg	768.51	J/mol×K	949.94	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=U382203&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