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

Inchi: InChI=1S/C22H40O6/c1-3-5-6-7-8-9-10-11-12-15-27-20(23)13-14-21(24)28-18-22(4-2)16
InchiKey: MOWXLPNHMBLFKT-UHFFFAOYSA-N
Formula: C22H40O6
SMILES: CCCCCCCCCCCOC(=O)CCC(=O)OCC1(CC)COCOC1
Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-486.76	kJ/mol	Joback Method
hf	-1181.45	kJ/mol	Joback Method
hfus	59.80	kJ/mol	Joback Method
hvap	91.18	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.785		Crippen Method
mcvol	336.600	ml/mol	McGowan Method
pc	1106.68	kPa	Joback Method
rinpol	2794.00		NIST Webbook
rinpol	2794.00		NIST Webbook
tb	929.03	K	Joback Method
tc	1138.36	K	Joback Method
tf	566.44	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1159.61	J/mol×K	929.03	Joback Method
cpg	1180.25	J/mol×K	963.92	Joback Method
cpg	1200.14	J/mol×K	998.81	Joback Method
cpg	1219.40	J/mol×K	1033.69	Joback Method
cpg	1238.13	J/mol×K	1068.58	Joback Method
cpg	1256.43	J/mol×K	1103.47	Joback Method
cpg	1274.41	J/mol×K	1138.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382212&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