Succinic acid, (5-ethyl-1,3-dioxan-5-yl)methyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H32O6/c1-5-7-15(14(3)4)24-17(20)9-8-16(19)23-12-18(6-2)10-21-13-22-11

InchiKey: JEUATORRIVATDY-UHFFFAOYSA-N

Formula: C18H32O6

SMILES: CCCC(OC(=O)CCC(=O)OCC1(CC)COCOC1)C(C)C

Mol. weight [g/mol]: 344.44

Physical Properties

Property code	Value	Unit	Source
gf	-525.32	kJ/mol	Joback Method
hf	-1109.45	kJ/mol	Joback Method
hfus	42.40	kJ/mol	Joback Method
hvap	81.50	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.078		Crippen Method
mcvol	280.240	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
rinpol	2241.00		NIST Webbook
rinpol	2241.00		NIST Webbook
tb	836.63	K	Joback Method
tc	1041.58	K	Joback Method
tf	491.36	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.21	J/mol×K	836.63	Joback Method
cpg	930.96	J/mol×K	870.79	Joback Method
cpg	948.93	J/mol×K	904.95	Joback Method
cpg	966.20	J/mol×K	939.10	Joback Method
cpg	982.85	J/mol×K	973.26	Joback Method
cpg	998.99	J/mol×K	1007.42	Joback Method
cpg	1014.69	J/mol×K	1041.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382207&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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