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

Inchi: InChI=1S/C23H42O6/c1-3-5-6-7-8-9-10-11-12-13-16-28-21(24)14-15-22(25)29-19-23(4-2
InchiKey: MOCYNKZQMQVSRP-UHFFFAOYSA-N
Formula: C23H42O6
SMILES: CCCCCCCCCCCCOC(=O)CCC(=O)OCC1(CC)COCOC1
Mol. weight [g/mol]: 414.58

Physical Properties

Property code	Value	Unit	Source
gf	-478.34	kJ/mol	Joback Method
hf	-1202.09	kJ/mol	Joback Method
hfus	62.39	kJ/mol	Joback Method
hvap	93.40	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	5.175		Crippen Method
mcvol	350.690	ml/mol	McGowan Method
pc	1039.24	kPa	Joback Method
rinpol	2897.00		NIST Webbook
tb	951.91	K	Joback Method
tc	1165.48	K	Joback Method
tf	577.71	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1223.73	J/mol×K	951.91	Joback Method
cpg	1245.09	J/mol×K	987.51	Joback Method
cpg	1265.70	J/mol×K	1023.10	Joback Method
cpg	1285.69	J/mol×K	1058.70	Joback Method
cpg	1305.15	J/mol×K	1094.29	Joback Method
cpg	1324.22	J/mol×K	1129.89	Joback Method
cpg	1342.99	J/mol×K	1165.48	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=U382213&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