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

Inchi: InChI=1S/C17H30O6/c1-3-5-6-7-10-22-15(18)8-9-16(19)23-13-17(4-2)11-20-14-21-12-17

InchiKey: ATFYRJWCGHHSCF-UHFFFAOYSA-N

Formula: C17H30O6

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

Mol. weight [g/mol]: 330.42

Physical Properties

Property code	Value	Unit	Source
gf	-528.86	kJ/mol	Joback Method
hf	-1078.25	kJ/mol	Joback Method
hfus	46.85	kJ/mol	Joback Method
hvap	80.05	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.834		Crippen Method
mcvol	266.150	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	2285.00		NIST Webbook
rinpol	2285.00		NIST Webbook
tb	814.63	K	Joback Method
tc	1015.48	K	Joback Method
tf	510.09	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.37	J/mol×K	814.63	Joback Method
cpg	869.35	J/mol×K	848.10	Joback Method
cpg	886.59	J/mol×K	881.58	Joback Method
cpg	903.17	J/mol×K	915.05	Joback Method
cpg	919.18	J/mol×K	948.53	Joback Method
cpg	934.70	J/mol×K	982.00	Joback Method
cpg	949.79	J/mol×K	1015.48	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382208&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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