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

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

InchiKey: BCJGZIPWPIFULM-UHFFFAOYSA-N

Formula: C18H32O6

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

Mol. weight [g/mol]: 344.44

Physical Properties

Property code	Value	Unit	Source
gf	-520.44	kJ/mol	Joback Method
hf	-1098.89	kJ/mol	Joback Method
hfus	49.45	kJ/mol	Joback Method
hvap	82.27	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.224		Crippen Method
mcvol	280.240	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	2382.00		NIST Webbook
rinpol	2382.00		NIST Webbook
tb	837.51	K	Joback Method
tc	1038.55	K	Joback Method
tf	521.36	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.23	J/mol×K	837.51	Joback Method
cpg	929.65	J/mol×K	871.02	Joback Method
cpg	947.34	J/mol×K	904.52	Joback Method
cpg	964.38	J/mol×K	938.03	Joback Method
cpg	980.85	J/mol×K	971.54	Joback Method
cpg	996.83	J/mol×K	1005.04	Joback Method
cpg	1012.41	J/mol×K	1038.55	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=U382209&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