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

Inchi: InChI=1S/C15H26O6/c1-4-15(8-18-11-19-9-15)10-21-14(17)6-5-13(16)20-7-12(2)3/h12H

InchiKey: LMOZJKVBOJUQKO-UHFFFAOYSA-N

Formula: C15H26O6

SMILES: CCC1(COC(=O)CCC(=O)OCC(C)C)COCOC1

Mol. weight [g/mol]: 302.36

Physical Properties

Property code	Value	Unit	Source
gf	-548.14	kJ/mol	Joback Method
hf	-1042.25	kJ/mol	Joback Method
hfus	38.15	kJ/mol	Joback Method
hvap	75.21	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.910		Crippen Method
mcvol	237.970	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	2038.00		NIST Webbook
tb	768.43	K	Joback Method
tc	973.58	K	Joback Method
tf	472.55	K	Joback Method
vc	0.890	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.23	J/mol×K	768.43	Joback Method
cpg	752.59	J/mol×K	802.62	Joback Method
cpg	769.17	J/mol×K	836.81	Joback Method
cpg	785.07	J/mol×K	871.00	Joback Method
cpg	800.36	J/mol×K	905.20	Joback Method
cpg	815.12	J/mol×K	939.39	Joback Method
cpg	829.42	J/mol×K	973.58	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=U382204&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