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

Inchi: InChI=1S/C19H34O6/c1-3-5-6-7-8-9-12-24-17(20)10-11-18(21)25-15-19(4-2)13-22-16-23

InchiKey: UUWYYYZWDPYOAX-UHFFFAOYSA-N

Formula: C19H34O6

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

Mol. weight [g/mol]: 358.47

Physical Properties

Property code	Value	Unit	Source
gf	-512.02	kJ/mol	Joback Method
hf	-1119.53	kJ/mol	Joback Method
hfus	52.04	kJ/mol	Joback Method
hvap	84.50	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.614		Crippen Method
mcvol	294.330	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
rinpol	2485.00		NIST Webbook
tb	860.39	K	Joback Method
tc	1062.32	K	Joback Method
tf	532.63	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.03	J/mol×K	860.39	Joback Method
cpg	990.93	J/mol×K	894.04	Joback Method
cpg	1009.09	J/mol×K	927.70	Joback Method
cpg	1026.61	J/mol×K	961.35	Joback Method
cpg	1043.57	J/mol×K	995.01	Joback Method
cpg	1060.05	J/mol×K	1028.66	Joback Method
cpg	1076.14	J/mol×K	1062.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382210&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