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

Inchi: InChI=1S/C16H28O6/c1-3-5-6-9-21-14(17)7-8-15(18)22-12-16(4-2)10-19-13-20-11-16/h3

InchiKey: PGIYOGUDGKZGLR-UHFFFAOYSA-N

Formula: C16H28O6

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

Mol. weight [g/mol]: 316.39

Physical Properties

Property code	Value	Unit	Source
gf	-537.28	kJ/mol	Joback Method
hf	-1057.61	kJ/mol	Joback Method
hfus	44.26	kJ/mol	Joback Method
hvap	77.82	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.444		Crippen Method
mcvol	252.060	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2185.00		NIST Webbook
rinpol	2185.00		NIST Webbook
tb	791.75	K	Joback Method
tc	993.05	K	Joback Method
tf	498.82	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.51	J/mol×K	791.75	Joback Method
cpg	810.06	J/mol×K	825.30	Joback Method
cpg	826.86	J/mol×K	858.85	Joback Method
cpg	843.01	J/mol×K	892.40	Joback Method
cpg	858.58	J/mol×K	925.95	Joback Method
cpg	873.64	J/mol×K	959.50	Joback Method
cpg	888.28	J/mol×K	993.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382206&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