

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

Inchi:	InChI=1S/C24H44O6/c1-3-5-6-7-8-9-10-11-12-13-14-17-29-22(25)15-16-23(26)30-20-24
InchiKey:	IMGFDOWUYLSNSQ-UHFFFAOYSA-N
Formula:	C24H44O6
SMILES:	CCCCCCCCCCCCCOC(=O)CCC(=O)OCC1(CC)COCOC1
Mol. weight [g/mol]:	428.60

Physical Properties

Property code	Value	Unit	Source
gf	-469.92	kJ/mol	Joback Method
hf	-1222.73	kJ/mol	Joback Method
hfus	64.98	kJ/mol	Joback Method
hvap	95.63	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.565		Crippen Method
mcvol	364.780	ml/mol	McGowan Method
pc	977.78	kPa	Joback Method
rinpol	2981.00		NIST Webbook
rinpol	2981.00		NIST Webbook
tb	974.79	K	Joback Method
tc	1193.61	K	Joback Method
tf	588.98	K	Joback Method
vc	1.401	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1288.58	J/molxK	974.79	Joback Method
cpg	1310.76	J/molxK	1011.26	Joback Method
cpg	1332.19	J/molxK	1047.73	Joback Method
cpg	1352.99	J/molxK	1084.20	Joback Method
cpg	1373.29	J/molxK	1120.67	Joback Method
cpg	1393.23	J/molxK	1157.14	Joback Method
cpg	1412.92	J/molxK	1193.61	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U382214&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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