Succinic acid, 3,7-dimethyloct-6-en-1-yl propyl ester

Inchi: InChI=1S/C17H30O4/c1-5-12-20-16(18)9-10-17(19)21-13-11-15(4)8-6-7-14(2)3/h7,15H,5

InchiKey: BLAINOUTIYVOOO-UHFFFAOYSA-N

Formula: C17H30O4

SMILES: CCCOC(=O)CCC(=O)OCCC(C)CCC=C(C)C

Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-306.35	kJ/mol	Joback Method
hf	-781.66	kJ/mol	Joback Method
hfus	40.73	kJ/mol	Joback Method
hvap	71.40	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.036		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
tb	744.54	K	Joback Method
tc	929.10	K	Joback Method
tf	391.63	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.43	J/mol×K	744.54	Joback Method
cpg	784.22	J/mol×K	775.30	Joback Method
cpg	800.11	J/mol×K	806.06	Joback Method
cpg	815.14	J/mol×K	836.82	Joback Method
cpg	829.32	J/mol×K	867.58	Joback Method
cpg	842.66	J/mol×K	898.34	Joback Method
cpg	855.19	J/mol×K	929.10	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=U353335&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