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

Inchi: InChI=1S/C26H48O4/c1-5-6-7-8-9-10-11-12-13-14-21-29-25(27)18-19-26(28)30-22-20-2

InchiKey: NZQUVKSTHQUHBY-UHFFFAOYSA-N

Formula: C26H48O4

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

Mol. weight [g/mol]: 424.66

Physical Properties

Property code	Value	Unit	Source
gf	-230.57	kJ/mol	Joback Method
hf	-967.42	kJ/mol	Joback Method
hfus	64.04	kJ/mol	Joback Method
hvap	91.43	kJ/mol	Joback Method
log10ws	-8.04		Crippen Method
logp	7.546		Crippen Method
mcvol	387.780	ml/mol	McGowan Method
pc	790.37	kPa	Joback Method
rinpol	2857.00		NIST Webbook
rinpol	2857.00		NIST Webbook
tb	950.46	K	Joback Method
tc	1166.63	K	Joback Method
tf	493.06	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1317.56	J/mol×K	950.46	Joback Method
cpg	1338.10	J/mol×K	986.49	Joback Method
cpg	1357.16	J/mol×K	1022.52	Joback Method
cpg	1374.79	J/mol×K	1058.54	Joback Method
cpg	1391.06	J/mol×K	1094.57	Joback Method
cpg	1406.04	J/mol×K	1130.60	Joback Method
cpg	1419.77	J/mol×K	1166.63	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=U353345&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