Succinic acid, 2-(adamant-1-yl)ethyl dec-2-yl ester

Inchi: InChI=1S/C26H44O4/c1-3-4-5-6-7-8-9-20(2)30-25(28)11-10-24(27)29-13-12-26-17-21-14

InchiKey: INTQLLOQZJGSNQ-UHFFFAOYSA-N

Formula: C26H44O4

SMILES: CCCCCCCCC(C)OC(=O)CCC(=O)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 420.63

Physical Properties

Property code	Value	Unit	Source
gf	-145.29	kJ/mol	Joback Method
hf	-867.71	kJ/mol	Joback Method
hfus	52.23	kJ/mol	Joback Method
hvap	89.84	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.599		Crippen Method
mcvol	359.500	ml/mol	McGowan Method
pc	984.55	kPa	Joback Method
rinpol	3100.00		NIST Webbook
tb	966.48	K	Joback Method
tc	1183.80	K	Joback Method
tf	582.06	K	Joback Method
vc	1.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.39	J/mol×K	966.48	Joback Method
cpg	1333.08	J/mol×K	1002.70	Joback Method
cpg	1357.51	J/mol×K	1038.92	Joback Method
cpg	1381.90	J/mol×K	1075.14	Joback Method
cpg	1406.43	J/mol×K	1111.36	Joback Method
cpg	1431.31	J/mol×K	1147.58	Joback Method
cpg	1456.75	J/mol×K	1183.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391369&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

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