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

Inchi: InChI=1S/C25H42O4/c1-3-4-5-6-7-8-9-19(2)29-24(27)11-10-23(26)28-18-25-15-20-12-21

InchiKey: BMHXZSILSKECKX-UHFFFAOYSA-N

Formula: C25H42O4

SMILES: CCCCCCCCC(C)OC(=O)CCC(=O)OCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 406.60

Physical Properties

Property code	Value	Unit	Source
gf	-153.71	kJ/mol	Joback Method
hf	-847.07	kJ/mol	Joback Method
hfus	49.63	kJ/mol	Joback Method
hvap	87.62	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.209		Crippen Method
mcvol	345.410	ml/mol	McGowan Method
pc	1046.65	kPa	Joback Method
rinpol	2944.00		NIST Webbook
tb	943.60	K	Joback Method
tc	1157.33	K	Joback Method
tf	570.79	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1242.28	J/mol×K	943.60	Joback Method
cpg	1265.99	J/mol×K	979.22	Joback Method
cpg	1289.38	J/mol×K	1014.84	Joback Method
cpg	1312.63	J/mol×K	1050.47	Joback Method
cpg	1335.94	J/mol×K	1086.09	Joback Method
cpg	1359.49	J/mol×K	1121.71	Joback Method
cpg	1383.48	J/mol×K	1157.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391359&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