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

Inchi: InChI=1S/C24H40O4/c1-3-5-6-18(4-2)17-28-23(26)8-7-22(25)27-10-9-24-14-19-11-20(15

InchiKey: OWSDIYFDCQZMLA-UHFFFAOYSA-N

Formula: C24H40O4

SMILES: CCCCC(CC)COC(=O)CCC(=O)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 392.57

Physical Properties

Property code	Value	Unit	Source
gf	-162.13	kJ/mol	Joback Method
hf	-826.43	kJ/mol	Joback Method
hfus	47.04	kJ/mol	Joback Method
hvap	85.39	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.676		Crippen Method
mcvol	331.320	ml/mol	McGowan Method
pc	1114.82	kPa	Joback Method
rinpol	2923.00		NIST Webbook
rinpol	2923.00		NIST Webbook
tb	920.72	K	Joback Method
tc	1131.78	K	Joback Method
tf	559.52	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1177.06	J/mol×K	920.72	Joback Method
cpg	1199.93	J/mol×K	955.90	Joback Method
cpg	1222.41	J/mol×K	991.07	Joback Method
cpg	1244.68	J/mol×K	1026.25	Joback Method
cpg	1266.92	J/mol×K	1061.43	Joback Method
cpg	1289.32	J/mol×K	1096.61	Joback Method
cpg	1312.05	J/mol×K	1131.78	Joback Method

Sources

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=U391367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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