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

Inchi: InChI=1S/C23H38O4/c1-3-5-6-17(4-2)15-26-21(24)7-8-22(25)27-16-23-12-18-9-19(13-23

InchiKey: VNVMFCUXYZOTRD-UHFFFAOYSA-N

Formula: C23H38O4

SMILES: CCCCC(CC)COC(=O)CCC(=O)OCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 378.55

Physical Properties

Property code	Value	Unit	Source
gf	-170.55	kJ/mol	Joback Method
hf	-805.79	kJ/mol	Joback Method
hfus	44.45	kJ/mol	Joback Method
hvap	83.17	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.286		Crippen Method
mcvol	317.230	ml/mol	McGowan Method
pc	1189.88	kPa	Joback Method
rinpol	2766.00		NIST Webbook
rinpol	2766.00		NIST Webbook
tb	897.84	K	Joback Method
tc	1107.10	K	Joback Method
tf	548.25	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1112.76	J/mol×K	897.84	Joback Method
cpg	1134.89	J/mol×K	932.72	Joback Method
cpg	1156.57	J/mol×K	967.59	Joback Method
cpg	1177.99	J/mol×K	1002.47	Joback Method
cpg	1199.30	J/mol×K	1037.35	Joback Method
cpg	1220.69	J/mol×K	1072.22	Joback Method
cpg	1242.32	J/mol×K	1107.10	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=U391357&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