Succinic acid, di((adamant-1-yl)methyl) ester

Inchi: InChI=1S/C26H38O4/c27-23(29-15-25-9-17-3-18(10-25)5-19(4-17)11-25)1-2-24(28)30-1
InchiKey: SVGWPLSOBPOCPF-UHFFFAOYSA-N
Formula: C26H38O4
SMILES: O=C(CCC(=O)OCC12CC3CC(CC(C3)C1)C2)OCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 414.58

Physical Properties

Property code	Value	Unit	Source
gf	14.10	kJ/mol	Joback Method
hf	-655.29	kJ/mol	Joback Method
hfus	42.83	kJ/mol	Joback Method
hvap	88.68	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.286		Crippen Method
mcvol	326.920	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
rinpol	3379.00		NIST Webbook
rinpol	3379.00		NIST Webbook
tb	986.98	K	Joback Method
tc	1222.04	K	Joback Method
tf	667.02	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1275.10	J/mol×K	986.98	Joback Method
cpg	1307.42	J/mol×K	1026.16	Joback Method
cpg	1341.35	J/mol×K	1065.33	Joback Method
cpg	1377.32	J/mol×K	1104.51	Joback Method
cpg	1415.80	J/mol×K	1143.69	Joback Method
cpg	1457.23	J/mol×K	1182.87	Joback Method
cpg	1502.06	J/mol×K	1222.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391360&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