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

Inchi: InChI=1S/C22H36O4/c1-3-4-5-6-16(2)26-21(24)8-7-20(23)25-15-22-12-17-9-18(13-22)11

InchiKey: ULGYLDSPRNGUAY-UHFFFAOYSA-N

Formula: C22H36O4

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

Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-178.97	kJ/mol	Joback Method
hf	-785.15	kJ/mol	Joback Method
hfus	41.86	kJ/mol	Joback Method
hvap	80.94	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.038		Crippen Method
mcvol	303.140	ml/mol	McGowan Method
pc	1272.78	kPa	Joback Method
rinpol	2635.00		NIST Webbook
rinpol	2635.00		NIST Webbook
tb	874.96	K	Joback Method
tc	1083.22	K	Joback Method
tf	536.98	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.38	J/mol×K	874.96	Joback Method
cpg	1070.87	J/mol×K	909.67	Joback Method
cpg	1091.87	J/mol×K	944.38	Joback Method
cpg	1112.53	J/mol×K	979.09	Joback Method
cpg	1133.03	J/mol×K	1013.80	Joback Method
cpg	1153.52	J/mol×K	1048.51	Joback Method
cpg	1174.18	J/mol×K	1083.22	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391356&Units=SI

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