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

Inchi: InChI=1S/C23H36O4/c24-21(6-7-22(25)27-16-17-4-2-1-3-5-17)26-9-8-23-13-18-10-19(14

InchiKey: NHANQUSNLYPBSN-UHFFFAOYSA-N

Formula: C23H36O4

SMILES: O=C(CCC(=O)OCC1CCCCC1)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-143.66	kJ/mol	Joback Method
hf	-746.19	kJ/mol	Joback Method
hfus	39.81	kJ/mol	Joback Method
hvap	83.98	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.040		Crippen Method
mcvol	306.370	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
rinpol	3040.00		NIST Webbook
rinpol	3040.00		NIST Webbook
tb	917.83	K	Joback Method
tc	1142.31	K	Joback Method
tf	570.63	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1110.47	J/mol×K	917.83	Joback Method
cpg	1133.78	J/mol×K	955.24	Joback Method
cpg	1156.58	J/mol×K	992.66	Joback Method
cpg	1179.08	J/mol×K	1030.07	Joback Method
cpg	1201.48	J/mol×K	1067.48	Joback Method
cpg	1224.01	J/mol×K	1104.89	Joback Method
cpg	1246.87	J/mol×K	1142.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391368&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