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

Inchi: InChI=1S/C22H34O4/c23-20(25-14-16-4-2-1-3-5-16)6-7-21(24)26-15-22-11-17-8-18(12-2

InchiKey: ONUFSWAIMVNJRO-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: O=C(CCC(=O)OCC12CC3CC(CC(C3)C1)C2)OCC1CCCCC1

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-152.08	kJ/mol	Joback Method
hf	-725.55	kJ/mol	Joback Method
hfus	37.22	kJ/mol	Joback Method
hvap	81.76	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.650		Crippen Method
mcvol	292.280	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
rinpol	2876.00		NIST Webbook
rinpol	2876.00		NIST Webbook
tb	894.95	K	Joback Method
tc	1120.41	K	Joback Method
tf	559.36	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1046.79	J/mol×K	894.95	Joback Method
cpg	1069.68	J/mol×K	932.53	Joback Method
cpg	1091.97	J/mol×K	970.10	Joback Method
cpg	1113.88	J/mol×K	1007.68	Joback Method
cpg	1135.62	J/mol×K	1045.26	Joback Method
cpg	1157.41	J/mol×K	1082.83	Joback Method
cpg	1179.46	J/mol×K	1120.41	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=U391358&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