Succinic acid, cyclohexylmethyl adamant-2-yl ester

Inchi: InChI=1S/C21H32O4/c22-19(24-13-14-4-2-1-3-5-14)6-7-20(23)25-21-17-9-15-8-16(11-17

InchiKey: FXYYPDGIDRCHAR-UHFFFAOYSA-N

Formula: C21H32O4

SMILES: O=C(CCC(=O)OC1C2CC3CC(C2)CC1C3)OCC1CCCCC1

Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-162.72	kJ/mol	Joback Method
hf	-740.49	kJ/mol	Joback Method
hfus	42.00	kJ/mol	Joback Method
hvap	80.37	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.258		Crippen Method
mcvol	278.190	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinpol	2806.00		NIST Webbook
rinpol	2806.00		NIST Webbook
tb	867.16	K	Joback Method
tc	1088.91	K	Joback Method
tf	519.95	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	990.31	J/mol×K	867.16	Joback Method
cpg	1078.76	J/mol×K	1051.95	Joback Method
cpg	1063.63	J/mol×K	1014.99	Joback Method
cpg	1047.32	J/mol×K	978.03	Joback Method
cpg	1029.73	J/mol×K	941.08	Joback Method
cpg	1010.76	J/mol×K	904.12	Joback Method
cpg	1092.81	J/mol×K	1088.91	Joback Method
dvisc	0.0017118	Pa×s	867.16	Joback Method

dvisc	0.0019084	Pa×s	809.29	Joback Method
dvisc	0.0021637	Pa×s	751.42	Joback Method
dvisc	0.0025050	Pa×s	693.56	Joback Method
dvisc	0.0029785	Pa×s	635.69	Joback Method
dvisc	0.0036665	Pa×s	577.82	Joback Method
dvisc	0.0047271	Pa×s	519.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391345&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
dvisc:	Dynamic viscosity
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