Succinic acid, 3-methylbut-2-yl adamant-2-yl ester

Inchi: InChI=1S/C19H30O4/c1-11(2)12(3)22-17(20)4-5-18(21)23-19-15-7-13-6-14(9-15)10-16(1

InchiKey: PWIRPKYRNGEDNO-UHFFFAOYSA-N

Formula: C19H30O4

SMILES: CC(C)C(C)OC(=O)CCC(=O)OC1C2CC3CC(C2)CC1C3

Mol. weight [g/mol]: 322.44

Physical Properties

Property code	Value	Unit	Source
gf	-208.89	kJ/mol	Joback Method
hf	-764.09	kJ/mol	Joback Method
hfus	37.94	kJ/mol	Joback Method
hvap	74.72	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.722		Crippen Method
mcvol	260.870	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinpol	2334.00		NIST Webbook
rinpol	2334.00		NIST Webbook
tb	800.97	K	Joback Method
tc	1008.01	K	Joback Method
tf	460.03	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.21	J/mol×K	800.97	Joback Method
cpg	892.69	J/mol×K	835.48	Joback Method
cpg	910.94	J/mol×K	869.98	Joback Method
cpg	928.04	J/mol×K	904.49	Joback Method
cpg	944.06	J/mol×K	939.00	Joback Method
cpg	959.08	J/mol×K	973.50	Joback Method
cpg	973.17	J/mol×K	1008.01	Joback Method
dvisc	0.0042462	Pa×s	460.03	Joback Method

dvisc	0.0032786	Pa×s	516.85	Joback Method
dvisc	0.0026645	Pa×s	573.68	Joback Method
dvisc	0.0022480	Pa×s	630.50	Joback Method
dvisc	0.0019506	Pa×s	687.32	Joback Method
dvisc	0.0017296	Pa×s	744.15	Joback Method
dvisc	0.0015601	Pa×s	800.97	Joback Method

Sources

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=U391340&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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