Succinic acid, cyclohexylmethyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C19H34O4/c1-15(12-19(2,3)4)13-22-17(20)10-11-18(21)23-14-16-8-6-5-7-9-16

InchiKey: BZYMIMLJHQJTOF-UHFFFAOYSA-N

Formula: C19H34O4

SMILES: CC(COC(=O)CCC(=O)OCC1CCCCC1)CC(C)(C)C

Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-333.89	kJ/mol	Joback Method
hf	-884.80	kJ/mol	Joback Method
hfus	31.44	kJ/mol	Joback Method
hvap	74.94	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.506		Crippen Method
mcvol	282.590	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
rinpol	2152.00		NIST Webbook
rinpol	2152.00		NIST Webbook
tb	802.58	K	Joback Method
tc	1005.59	K	Joback Method
tf	443.01	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.36	J/mol×K	802.58	Joback Method
cpg	926.64	J/mol×K	836.41	Joback Method
cpg	944.58	J/mol×K	870.25	Joback Method
cpg	961.22	J/mol×K	904.08	Joback Method
cpg	976.60	J/mol×K	937.92	Joback Method
cpg	990.76	J/mol×K	971.75	Joback Method
cpg	1003.74	J/mol×K	1005.59	Joback Method
dvisc	0.0012420	Pa×s	443.01	Joback Method

dvisc	0.0005198	Pa×s	502.94	Joback Method
dvisc	0.0002618	Pa×s	562.87	Joback Method
dvisc	0.0001505	Pa×s	622.79	Joback Method
dvisc	0.0000954	Pa×s	682.72	Joback Method
dvisc	0.0000650	Pa×s	742.65	Joback Method
dvisc	0.0000470	Pa×s	802.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389545&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