Succinic acid, di(2,4,4-trimethylpentyl) ester

Inchi: InChI=1S/C20H38O4/c1-15(11-19(3,4)5)13-23-17(21)9-10-18(22)24-14-16(2)12-20(6,7)8
InchiKey: UPELHNUPBADRJV-UHFFFAOYSA-N
Formula: C20H38O4
SMILES: CC(COC(=O)CCC(=O)OCC(C)CC(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]: 342.51

Physical Properties

Property code	Value	Unit	Source
gf	-349.52	kJ/mol	Joback Method
hf	-973.79	kJ/mol	Joback Method
hfus	31.26	kJ/mol	Joback Method
hvap	75.06	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.998		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	802.24	K	Joback Method
tc	994.46	K	Joback Method
tf	434.32	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.22	J/mol×K	802.24	Joback Method
cpg	990.84	J/mol×K	834.28	Joback Method
cpg	1008.33	J/mol×K	866.31	Joback Method
cpg	1024.74	J/mol×K	898.35	Joback Method
cpg	1040.11	J/mol×K	930.39	Joback Method
cpg	1054.51	J/mol×K	962.43	Joback Method
cpg	1067.96	J/mol×K	994.46	Joback Method
dvisc	0.0011509	Pa×s	434.32	Joback Method

dvisc	0.0004263	Pa×s	495.64	Joback Method
dvisc	0.0001965	Pa×s	556.96	Joback Method
dvisc	0.0001056	Pa×s	618.28	Joback Method
dvisc	0.0000635	Pa×s	679.60	Joback Method
dvisc	0.0000415	Pa×s	740.92	Joback Method
dvisc	0.0000290	Pa×s	802.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381334&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