di-(1,3-Dimethylbutyl)suberate

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

Physical Properties

Property code	Value	Unit	Source
gf	-360.08	kJ/mol	Joback Method
hf	-966.85	kJ/mol	Joback Method
hfus	39.04	kJ/mol	Joback Method
hvap	76.87	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.283		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1100.81	kPa	Joback Method
rinpol	2062.00		NIST Webbook
rinpol	2062.00		NIST Webbook
tb	807.82	K	Joback Method
tc	995.23	K	Joback Method
tf	399.48	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.09	J/mol×K	807.82	Joback Method
cpg	989.72	J/mol×K	839.05	Joback Method
cpg	1007.22	J/mol×K	870.29	Joback Method
cpg	1023.63	J/mol×K	901.52	Joback Method
cpg	1038.95	J/mol×K	932.76	Joback Method
cpg	1053.20	J/mol×K	963.99	Joback Method
cpg	1066.41	J/mol×K	995.23	Joback Method
dvisc	0.0018698	Pa×s	399.48	Joback Method

dvisc	0.0006083	Pa×s	467.54	Joback Method
dvisc	0.0002633	Pa×s	535.59	Joback Method
dvisc	0.0001376	Pa×s	603.65	Joback Method
dvisc	0.0000821	Pa×s	671.71	Joback Method
dvisc	0.0000538	Pa×s	739.76	Joback Method
dvisc	0.0000379	Pa×s	807.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541636&Units=SI

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