Sebacic acid, dineopentyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-344.64	kJ/mol	Joback Method
hf	-963.23	kJ/mol	Joback Method
hfus	38.30	kJ/mol	Joback Method
hvap	75.83	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	5.286		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
rinpol	2216.00		NIST Webbook
tb	803.12	K	Joback Method
tc	992.21	K	Joback Method
tf	464.32	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.25	J/mol×K	803.12	Joback Method
cpg	1052.53	J/mol×K	960.69	Joback Method
cpg	1038.24	J/mol×K	929.18	Joback Method
cpg	1023.01	J/mol×K	897.66	Joback Method
cpg	1006.80	J/mol×K	866.15	Joback Method
cpg	989.56	J/mol×K	834.63	Joback Method
cpg	1065.94	J/mol×K	992.21	Joback Method
dvisc	0.0000343	Pa×s	803.12	Joback Method
dvisc	0.0000473	Pa×s	746.65	Joback Method

dvisc	0.0000687	Pa×s	690.19	Joback Method
dvisc	0.0001068	Pa×s	633.72	Joback Method
dvisc	0.0001808	Pa×s	577.25	Joback Method
dvisc	0.0003431	Pa×s	520.79	Joback Method
dvisc	0.0007610	Pa×s	464.32	Joback Method

Sources

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=U354479&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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