Sebacic acid, neopentyl pentyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-347.48	kJ/mol	Joback Method
hf	-954.48	kJ/mol	Joback Method
hfus	45.72	kJ/mol	Joback Method
hvap	77.13	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.430		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	2321.00		NIST Webbook
rinpol	2321.00		NIST Webbook
tb	806.35	K	Joback Method
tc	992.19	K	Joback Method
tf	461.90	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.19	J/mol×K	806.35	Joback Method
cpg	1051.16	J/mol×K	961.22	Joback Method
cpg	1036.94	J/mol×K	930.24	Joback Method
cpg	1021.76	J/mol×K	899.27	Joback Method
cpg	1005.60	J/mol×K	868.30	Joback Method
cpg	988.42	J/mol×K	837.32	Joback Method
cpg	1064.44	J/mol×K	992.19	Joback Method
dvisc	0.0000427	Pa×s	806.35	Joback Method

dvisc	0.0000577	Pa×s	748.94	Joback Method
dvisc	0.0000820	Pa×s	691.53	Joback Method
dvisc	0.0001242	Pa×s	634.12	Joback Method
dvisc	0.0002043	Pa×s	576.72	Joback Method
dvisc	0.0003752	Pa×s	519.31	Joback Method
dvisc	0.0008014	Pa×s	461.90	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=U354466&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