Sebacic acid, 2,4-dimethylpent-3-yl propyl ester

Inchi: InChI=1S/C20H38O4/c1-6-15-23-18(21)13-11-9-7-8-10-12-14-19(22)24-20(16(2)3)17(4)5

InchiKey: UVGKBFPMQWWZAV-UHFFFAOYSA-N

Formula: C20H38O4

SMILES: CCCOC(=O)CCCCCCCCC(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 342.51

Physical Properties

Property code	Value	Unit	Source
gf	-357.64	kJ/mol	Joback Method
hf	-961.57	kJ/mol	Joback Method
hfus	42.56	kJ/mol	Joback Method
hvap	77.26	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.284		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1094.99	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2238.00		NIST Webbook
tb	808.26	K	Joback Method
tc	994.56	K	Joback Method
tf	414.48	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.62	J/mol×K	808.26	Joback Method
cpg	989.13	J/mol×K	839.31	Joback Method
cpg	1006.54	J/mol×K	870.36	Joback Method
cpg	1022.88	J/mol×K	901.41	Joback Method
cpg	1038.15	J/mol×K	932.46	Joback Method
cpg	1052.38	J/mol×K	963.51	Joback Method
cpg	1065.59	J/mol×K	994.56	Joback Method
dvisc	0.0014761	Pa×s	414.48	Joback Method

dvisc	0.0005410	Pa×s	480.11	Joback Method
dvisc	0.0002524	Pa×s	545.74	Joback Method
dvisc	0.0001387	Pa×s	611.37	Joback Method
dvisc	0.0000856	Pa×s	677.00	Joback Method
dvisc	0.0000575	Pa×s	742.63	Joback Method
dvisc	0.0000412	Pa×s	808.26	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=U355424&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