Sebacic acid, pent-4-en-2-yl pentyl ester

Inchi: InChI=1S/C20H36O4/c1-4-6-13-17-23-19(21)15-11-9-7-8-10-12-16-20(22)24-18(3)14-5-2
InchiKey: HKCPBOLULPOOGU-UHFFFAOYSA-N
Formula: C20H36O4
SMILES: C=CCC(C)OC(=O)CCCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-264.92	kJ/mol	Joback Method
hf	-825.58	kJ/mol	Joback Method
hfus	48.33	kJ/mol	Joback Method
hvap	77.37	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.348		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1114.08	kPa	Joback Method
rinpol	2301.00		NIST Webbook
tb	805.82	K	Joback Method
tc	990.69	K	Joback Method
tf	442.72	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.73	J/mol×K	805.82	Joback Method
cpg	1021.64	J/mol×K	959.88	Joback Method
cpg	1007.82	J/mol×K	929.06	Joback Method
cpg	993.04	J/mol×K	898.25	Joback Method
cpg	977.28	J/mol×K	867.44	Joback Method
cpg	960.52	J/mol×K	836.63	Joback Method
cpg	1034.51	J/mol×K	990.69	Joback Method
dvisc	0.0000522	Pa×s	805.82	Joback Method
dvisc	0.0000700	Pa×s	745.30	Joback Method

dvisc	0.0000987	Pa×s	684.79	Joback Method
dvisc	0.0001489	Pa×s	624.27	Joback Method
dvisc	0.0002452	Pa×s	563.75	Joback Method
dvisc	0.0004555	Pa×s	503.24	Joback Method
dvisc	0.0010021	Pa×s	442.72	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=U355951&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