Sebacic acid, undecyl pent-4-enyl ester

Inchi: InChI=1S/C26H48O4/c1-3-5-7-8-9-10-13-16-20-24-30-26(28)22-18-15-12-11-14-17-21-2
InchiKey: RIEUSUJNYDBBPL-UHFFFAOYSA-N
Formula: C26H48O4
SMILES: C=CCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 424.66

Physical Properties

Property code	Value	Unit	Source
gf	-211.96	kJ/mol	Joback Method
hf	-944.14	kJ/mol	Joback Method
hfus	67.39	kJ/mol	Joback Method
hvap	91.11	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.691		Crippen Method
mcvol	387.780	ml/mol	McGowan Method
pc	780.25	kPa	Joback Method
rinpol	2985.00		NIST Webbook
tb	943.54	K	Joback Method
tc	1160.67	K	Joback Method
tf	525.34	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.55	J/mol×K	943.54	Joback Method
cpg	1336.29	J/mol×K	979.73	Joback Method
cpg	1355.46	J/mol×K	1015.92	Joback Method
cpg	1373.10	J/mol×K	1052.11	Joback Method
cpg	1389.28	J/mol×K	1088.30	Joback Method
cpg	1404.04	J/mol×K	1124.48	Joback Method
cpg	1417.43	J/mol×K	1160.67	Joback Method
dvisc	0.0004211	Pa×s	525.34	Joback Method
dvisc	0.0001960	Pa×s	595.04	Joback Method

dvisc	0.0001071	Pa×s	664.74	Joback Method
dvisc	0.0000656	Pa×s	734.44	Joback Method
dvisc	0.0000438	Pa×s	804.14	Joback Method
dvisc	0.0000312	Pa×s	873.84	Joback Method
dvisc	0.0000233	Pa×s	943.54	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=U355417&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