Sebacic acid, heptyl tetradec-2-enyl ester

Inchi: InChI=1S/C31H58O4/c1-3-5-7-9-10-11-12-13-14-17-21-25-29-35-31(33)27-23-19-16-15-
InchiKey: NRSSTKBTRHZGFP-NJNXFGOHSA-N
Formula: C31H58O4
SMILES: CCCCCCCCCCCC=CCOC(=O)CCCCCCCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 494.79

Physical Properties

Property code	Value	Unit	Source
gf	-177.48	kJ/mol	Joback Method
hf	-1055.55	kJ/mol	Joback Method
hfus	81.82	kJ/mol	Joback Method
hvap	102.87	kJ/mol	Joback Method
log10ws	-10.38		Crippen Method
logp	9.641		Crippen Method
mcvol	458.230	ml/mol	McGowan Method
pc	609.66	kPa	Joback Method
rinpol	3514.00		NIST Webbook
rinpol	3514.00		NIST Webbook
tb	1065.42	K	Joback Method
tc	1343.17	K	Joback Method
tf	578.37	K	Joback Method
vc	1.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1642.56	J/mol×K	1065.42	Joback Method
cpg	1667.34	J/mol×K	1111.71	Joback Method
cpg	1689.72	J/mol×K	1158.00	Joback Method
cpg	1709.85	J/mol×K	1204.29	Joback Method
cpg	1727.91	J/mol×K	1250.59	Joback Method
cpg	1744.05	J/mol×K	1296.88	Joback Method
cpg	1758.45	J/mol×K	1343.17	Joback Method
dvisc	0.0001934	Pa×s	578.37	Joback Method

dvisc	0.0000836	Pa×s	659.54	Joback Method
dvisc	0.0000434	Pa×s	740.72	Joback Method
dvisc	0.0000257	Pa×s	821.89	Joback Method
dvisc	0.0000167	Pa×s	903.07	Joback Method
dvisc	0.0000116	Pa×s	984.25	Joback Method
dvisc	0.0000086	Pa×s	1065.42	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=U355403&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