Sebacic acid, 4-methoxy-2-methylbutyl tetradecyl ester

Other names: Sebacic acid, 4-methoxy-2-methylphenyl tetradecyl ester
Inchi: InChI=1S/C30H58O5/c1-4-5-6-7-8-9-10-11-12-15-18-21-25-34-29(31)22-19-16-13-14-17
InchiKey: DTEVRIYOBVBQOM-UHFFFAOYSA-N
Formula: C30H58O5
SMILES: CCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(C)CCOC
Mol. weight [g/mol]: 498.78

Physical Properties

Property code	Value	Unit	Source
gf	-373.56	kJ/mol	Joback Method
hf	-1289.63	kJ/mol	Joback Method
hfus	76.69	kJ/mol	Joback Method
hvap	102.71	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	8.567		Crippen Method
mcvol	454.310	ml/mol	McGowan Method
pc	620.34	kPa	Joback Method
rinpol	3463.00		NIST Webbook
tb	1060.36	K	Joback Method
tc	1338.15	K	Joback Method
tf	579.41	K	Joback Method
vc	1.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1635.89	J/mol×K	1060.36	Joback Method
cpg	1658.96	J/mol×K	1106.66	Joback Method
cpg	1679.04	J/mol×K	1152.96	Joback Method
cpg	1696.21	J/mol×K	1199.25	Joback Method
cpg	1710.56	J/mol×K	1245.55	Joback Method
cpg	1722.21	J/mol×K	1291.85	Joback Method
cpg	1731.24	J/mol×K	1338.15	Joback Method
dvisc	0.0001777	Pa×s	579.41	Joback Method

dvisc	0.0000763	Pa×s	659.57	Joback Method
dvisc	0.0000393	Pa×s	739.73	Joback Method
dvisc	0.0000231	Pa×s	819.88	Joback Method
dvisc	0.0000149	Pa×s	900.04	Joback Method
dvisc	0.0000103	Pa×s	980.20	Joback Method
dvisc	0.0000076	Pa×s	1060.36	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=U355334&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