Sebacic acid, 2-decyl dodecyl ester

Inchi: InChI=1S/C32H62O4/c1-4-6-8-10-12-13-14-17-21-25-29-35-31(33)27-23-19-15-16-20-24
InchiKey: AYBBQRVTSNUXDS-UHFFFAOYSA-N
Formula: C32H62O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(C)CCCCCCCC
Mol. weight [g/mol]: 510.83

Physical Properties

Property code	Value	Unit	Source
gf	-251.72	kJ/mol	Joback Method
hf	-1198.69	kJ/mol	Joback Method
hfus	80.69	kJ/mol	Joback Method
hvap	104.75	kJ/mol	Joback Method
log10ws	-11.05		Crippen Method
logp	10.254		Crippen Method
mcvol	476.620	ml/mol	McGowan Method
pc	569.60	kPa	Joback Method
rinpol	3477.00		NIST Webbook
tb	1083.70	K	Joback Method
tc	1379.80	K	Joback Method
tf	579.72	K	Joback Method
vc	1.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1736.88	J/mol×K	1083.70	Joback Method
cpg	1762.49	J/mol×K	1133.05	Joback Method
cpg	1784.99	J/mol×K	1182.40	Joback Method
cpg	1804.54	J/mol×K	1231.75	Joback Method
cpg	1821.32	J/mol×K	1281.10	Joback Method
cpg	1835.51	J/mol×K	1330.45	Joback Method
cpg	1847.27	J/mol×K	1379.80	Joback Method
dvisc	0.0002008	Pa×s	579.72	Joback Method
dvisc	0.0000821	Pa×s	663.72	Joback Method

dvisc	0.0000410	Pa×s	747.71	Joback Method
dvisc	0.0000236	Pa×s	831.71	Joback Method
dvisc	0.0000150	Pa×s	915.71	Joback Method
dvisc	0.0000103	Pa×s	999.70	Joback Method
dvisc	0.0000075	Pa×s	1083.70	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=U355495&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