Sebacic acid, 4-heptyl pentadecyl ester

Inchi: InChI=1S/C32H62O4/c1-4-7-8-9-10-11-12-13-14-15-18-21-24-29-35-31(33)27-22-19-16-
InchiKey: OMCIGESDBIVKGG-UHFFFAOYSA-N
Formula: C32H62O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(CCC)CCC
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	3452.00		NIST Webbook
rinpol	3452.00		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:	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=U355395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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