Sebacic acid, 2,4-dimethylpent-3-yl pentadecyl ester

Inchi: InChI=1S/C32H62O4/c1-6-7-8-9-10-11-12-13-14-15-18-21-24-27-35-30(33)25-22-19-16-

InchiKey: IQDRZKWTALQNIE-UHFFFAOYSA-N

Formula: C32H62O4

SMILES: CCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 510.83

Physical Properties

Property code	Value	Unit	Source
gf	-256.60	kJ/mol	Joback Method
hf	-1209.25	kJ/mol	Joback Method
hfus	73.64	kJ/mol	Joback Method
hvap	103.97	kJ/mol	Joback Method
log10ws	-10.57		Crippen Method
logp	9.965		Crippen Method
mcvol	476.620	ml/mol	McGowan Method
pc	573.98	kPa	Joback Method
rinpol	3437.00		NIST Webbook
tb	1082.82	K	Joback Method
tc	1370.02	K	Joback Method
tf	549.72	K	Joback Method
vc	1.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1737.08	J/mol×K	1082.82	Joback Method
cpg	1761.73	J/mol×K	1130.69	Joback Method
cpg	1783.41	J/mol×K	1178.55	Joback Method
cpg	1802.25	J/mol×K	1226.42	Joback Method
cpg	1818.43	J/mol×K	1274.29	Joback Method
cpg	1832.09	J/mol×K	1322.15	Joback Method
cpg	1843.40	J/mol×K	1370.02	Joback Method
dvisc	0.0002592	Pa×s	549.72	Joback Method
dvisc	0.0000901	Pa×s	638.57	Joback Method

dvisc	0.0000406	Pa×s	727.42	Joback Method
dvisc	0.0000217	Pa×s	816.27	Joback Method
dvisc	0.0000132	Pa×s	905.12	Joback Method
dvisc	0.0000087	Pa×s	993.97	Joback Method
dvisc	0.0000062	Pa×s	1082.82	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=U355437&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

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