Sebacic acid, 3,3-dimethylbut-2-yl hexadecyl ester

Inchi: InChI=1S/C32H62O4/c1-6-7-8-9-10-11-12-13-14-15-16-19-22-25-28-35-30(33)26-23-20-

InchiKey: YMUMDAXINCWASP-UHFFFAOYSA-N

Formula: C32H62O4

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

Mol. weight [g/mol]: 510.83

Physical Properties

Property code	Value	Unit	Source
gf	-248.88	kJ/mol	Joback Method
hf	-1207.44	kJ/mol	Joback Method
hfus	73.27	kJ/mol	Joback Method
hvap	103.45	kJ/mol	Joback Method
log10ws	-10.81		Crippen Method
logp	10.109		Crippen Method
mcvol	476.620	ml/mol	McGowan Method
pc	574.80	kPa	Joback Method
rinpol	3461.00		NIST Webbook
rinpol	3461.00		NIST Webbook
tb	1080.47	K	Joback Method
tc	1363.10	K	Joback Method
tf	582.14	K	Joback Method
vc	1.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1736.71	J/mol×K	1080.47	Joback Method
cpg	1761.88	J/mol×K	1127.57	Joback Method
cpg	1784.50	J/mol×K	1174.68	Joback Method
cpg	1804.77	J/mol×K	1221.78	Joback Method
cpg	1822.90	J/mol×K	1268.89	Joback Method
cpg	1839.08	J/mol×K	1315.99	Joback Method
cpg	1853.50	J/mol×K	1363.10	Joback Method
dvisc	0.0001728	Pa×s	582.14	Joback Method

dvisc	0.0000681	Pa×s	665.19	Joback Method
dvisc	0.0000330	Pa×s	748.25	Joback Method
dvisc	0.0000185	Pa×s	831.31	Joback Method
dvisc	0.0000115	Pa×s	914.36	Joback Method
dvisc	0.0000078	Pa×s	997.41	Joback Method
dvisc	0.0000056	Pa×s	1080.47	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=U355610&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