Adipic acid, 3,3-dimethylbut-2-yl eicosyl ester

Inchi: InChI=1S/C32H62O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-28-35-30(
InchiKey: JHRRSNSZJRVYCY-UHFFFAOYSA-N
Formula: C32H62O4
SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)CCCCC(=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	3411.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353683&Units=SI
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

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