Diethylmalonic acid, 3-methylpent-2-yl octadecyl ester

Inchi: InChI=1S/C31H60O4/c1-7-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-34-29(32)
InchiKey: SGDZDPNGPOAUIP-UHFFFAOYSA-N
Formula: C31H60O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)C(C)CC
Mol. weight [g/mol]: 496.81

Physical Properties

Property code	Value	Unit	Source
gf	-259.74	kJ/mol	Joback Method
hf	-1192.08	kJ/mol	Joback Method
hfus	67.16	kJ/mol	Joback Method
hvap	100.84	kJ/mol	Joback Method
log10ws	-10.15		Crippen Method
logp	9.575		Crippen Method
mcvol	462.530	ml/mol	McGowan Method
pc	604.58	kPa	Joback Method
rinpol	3090.00		NIST Webbook
tb	1057.15	K	Joback Method
tc	1321.25	K	Joback Method
tf	555.87	K	Joback Method
vc	1.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1670.88	J/mol×K	1057.15	Joback Method
cpg	1694.76	J/mol×K	1101.17	Joback Method
cpg	1716.36	J/mol×K	1145.18	Joback Method
cpg	1735.83	J/mol×K	1189.20	Joback Method
cpg	1753.35	J/mol×K	1233.22	Joback Method
cpg	1769.04	J/mol×K	1277.23	Joback Method
cpg	1783.08	J/mol×K	1321.25	Joback Method
dvisc	0.0002305	Pa×s	555.87	Joback Method
dvisc	0.0000842	Pa×s	639.42	Joback Method

dvisc	0.0000389	Pa×s	722.96	Joback Method
dvisc	0.0000210	Pa×s	806.51	Joback Method
dvisc	0.0000128	Pa×s	890.06	Joback Method
dvisc	0.0000085	Pa×s	973.60	Joback Method
dvisc	0.0000060	Pa×s	1057.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369743&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