Diethylmalonic acid, heptadecyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C32H62O4/c1-8-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-35-29(33)32(
InchiKey: LBCYZAPGDKWPNV-UHFFFAOYSA-N
Formula: C32H62O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]: 510.83

Physical Properties

Property code	Value	Unit	Source
gf	-246.04	kJ/mol	Joback Method
hf	-1216.19	kJ/mol	Joback Method
hfus	65.86	kJ/mol	Joback Method
hvap	102.16	kJ/mol	Joback Method
log10ws	-10.22		Crippen Method
logp	9.823		Crippen Method
mcvol	476.620	ml/mol	McGowan Method
pc	580.08	kPa	Joback Method
rinpol	3136.00		NIST Webbook
rinpol	3136.00		NIST Webbook
tb	1077.24	K	Joback Method
tc	1348.31	K	Joback Method
tf	584.56	K	Joback Method
vc	1.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1736.49	J/mol×K	1077.24	Joback Method
cpg	1761.25	J/mol×K	1122.42	Joback Method
cpg	1783.94	J/mol×K	1167.60	Joback Method
cpg	1804.78	J/mol×K	1212.77	Joback Method
cpg	1823.97	J/mol×K	1257.95	Joback Method
cpg	1841.72	J/mol×K	1303.13	Joback Method
cpg	1858.26	J/mol×K	1348.31	Joback Method
dvisc	0.0001482	Pa×s	584.56	Joback Method

dvisc	0.0000565	Pa×s	666.67	Joback Method
dvisc	0.0000266	Pa×s	748.79	Joback Method
dvisc	0.0000145	Pa×s	830.90	Joback Method
dvisc	0.0000089	Pa×s	913.01	Joback Method
dvisc	0.0000059	Pa×s	995.13	Joback Method
dvisc	0.0000041	Pa×s	1077.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369489&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

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