Malonic acid, 2,4-dimethylpent-3-yl octadecyl ester

Inchi: InChI=1S/C28H54O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-31-26(29)23-
InchiKey: HRNPHWZEAGUFIY-UHFFFAOYSA-N
Formula: C28H54O4
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 454.73

Physical Properties

Property code	Value	Unit	Source
gf	-290.28	kJ/mol	Joback Method
hf	-1126.69	kJ/mol	Joback Method
hfus	63.28	kJ/mol	Joback Method
hvap	95.07	kJ/mol	Joback Method
log10ws	-8.90		Crippen Method
logp	8.405		Crippen Method
mcvol	420.260	ml/mol	McGowan Method
pc	696.18	kPa	Joback Method
rinpol	2977.00		NIST Webbook
rinpol	2977.00		NIST Webbook
tb	991.30	K	Joback Method
tc	1224.98	K	Joback Method
tf	504.64	K	Joback Method
vc	1.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.44	J/mol×K	991.30	Joback Method
cpg	1497.42	J/mol×K	1030.25	Joback Method
cpg	1517.40	J/mol×K	1069.19	Joback Method
cpg	1535.48	J/mol×K	1108.14	Joback Method
cpg	1551.71	J/mol×K	1147.09	Joback Method
cpg	1566.16	J/mol×K	1186.03	Joback Method
cpg	1578.90	J/mol×K	1224.98	Joback Method
dvisc	0.0004778	Pa×s	504.64	Joback Method

dvisc	0.0001686	Pa×s	585.75	Joback Method
dvisc	0.0000766	Pa×s	666.86	Joback Method
dvisc	0.0000413	Pa×s	747.97	Joback Method
dvisc	0.0000252	Pa×s	829.08	Joback Method
dvisc	0.0000167	Pa×s	910.19	Joback Method
dvisc	0.0000119	Pa×s	991.30	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=U349024&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