Dimethylmalonic acid, heptadecyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C28H54O4/c1-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-31-26(29)28(5

InchiKey: OMHOVWRMNJXIKB-UHFFFAOYSA-N

Formula: C28H54O4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OC(CC)C(C)C

Mol. weight [g/mol]: 454.73

Physical Properties

Property code	Value	Unit	Source
gf	-285.00	kJ/mol	Joback Method
hf	-1130.16	kJ/mol	Joback Method
hfus	59.39	kJ/mol	Joback Method
hvap	94.16	kJ/mol	Joback Method
log10ws	-8.90		Crippen Method
logp	8.405		Crippen Method
mcvol	420.260	ml/mol	McGowan Method
pc	700.24	kPa	Joback Method
rinpol	2859.00		NIST Webbook
tb	988.51	K	Joback Method
tc	1218.05	K	Joback Method
tf	522.06	K	Joback Method
vc	1.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.73	J/mol×K	988.51	Joback Method
cpg	1496.50	J/mol×K	1026.77	Joback Method
cpg	1516.51	J/mol×K	1065.02	Joback Method
cpg	1534.84	J/mol×K	1103.28	Joback Method
cpg	1551.60	J/mol×K	1141.54	Joback Method
cpg	1566.86	J/mol×K	1179.79	Joback Method
cpg	1580.72	J/mol×K	1218.05	Joback Method
dvisc	0.0003674	Pa×s	522.06	Joback Method
dvisc	0.0001361	Pa×s	599.80	Joback Method

dvisc	0.0000633	Pa×s	677.54	Joback Method
dvisc	0.0000345	Pa×s	755.29	Joback Method
dvisc	0.0000210	Pa×s	833.03	Joback Method
dvisc	0.0000140	Pa×s	910.77	Joback Method
dvisc	0.0000099	Pa×s	988.51	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=U361802&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