Dimethylmalonic acid, octyl 3-phenylpropyl ester

Inchi: InChI=1S/C22H34O4/c1-4-5-6-7-8-12-17-25-20(23)22(2,3)21(24)26-18-13-16-19-14-10-9

InchiKey: SORGGFCODMJBMX-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: CCCCCCCCOC(=O)C(C)(C)C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-218.23	kJ/mol	Joback Method
hf	-759.23	kJ/mol	Joback Method
hfus	44.94	kJ/mol	Joback Method
hvap	83.86	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.092		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1198.96	kPa	Joback Method
rinpol	2422.00		NIST Webbook
tb	878.79	K	Joback Method
tc	1084.30	K	Joback Method
tf	510.86	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.42	J/mol×K	878.79	Joback Method
cpg	1015.14	J/mol×K	913.04	Joback Method
cpg	1030.66	J/mol×K	947.29	Joback Method
cpg	1045.03	J/mol×K	981.54	Joback Method
cpg	1058.30	J/mol×K	1015.79	Joback Method
cpg	1070.52	J/mol×K	1050.05	Joback Method
cpg	1081.75	J/mol×K	1084.30	Joback Method
dvisc	0.0005115	Pa×s	510.86	Joback Method
dvisc	0.0002510	Pa×s	572.18	Joback Method

dvisc	0.0001414	Pa×s	633.50	Joback Method
dvisc	0.0000882	Pa×s	694.83	Joback Method
dvisc	0.0000593	Pa×s	756.15	Joback Method
dvisc	0.0000424	Pa×s	817.47	Joback Method
dvisc	0.0000317	Pa×s	878.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361837&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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