Dimethylmalonic acid, heptyl 2-phenethyl ester

Inchi: InChI=1S/C20H30O4/c1-4-5-6-7-11-15-23-18(21)20(2,3)19(22)24-16-14-17-12-9-8-10-13

InchiKey: JMCJZWAZIMUGMS-UHFFFAOYSA-N

Formula: C20H30O4

SMILES: CCCCCCCOC(=O)C(C)(C)C(=O)OCCc1ccccc1

Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-235.07	kJ/mol	Joback Method
hf	-717.95	kJ/mol	Joback Method
hfus	39.76	kJ/mol	Joback Method
hvap	79.41	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.312		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1375.82	kPa	Joback Method
rinpol	2214.00		NIST Webbook
tb	833.03	K	Joback Method
tc	1037.37	K	Joback Method
tf	488.32	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.40	J/mol×K	833.03	Joback Method
cpg	895.78	J/mol×K	867.09	Joback Method
cpg	911.01	J/mol×K	901.14	Joback Method
cpg	925.14	J/mol×K	935.20	Joback Method
cpg	938.20	J/mol×K	969.25	Joback Method
cpg	950.26	J/mol×K	1003.31	Joback Method
cpg	961.35	J/mol×K	1037.37	Joback Method
dvisc	0.0006491	Pa×s	488.32	Joback Method
dvisc	0.0003253	Pa×s	545.77	Joback Method

dvisc	0.0001860	Pa×s	603.22	Joback Method
dvisc	0.0001172	Pa×s	660.67	Joback Method
dvisc	0.0000795	Pa×s	718.13	Joback Method
dvisc	0.0000571	Pa×s	775.58	Joback Method
dvisc	0.0000430	Pa×s	833.03	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=U361619&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