Dimethylmalonic acid, heptyl 3-phenylpropyl ester

Inchi: InChI=1S/C21H32O4/c1-4-5-6-7-11-16-24-19(22)21(2,3)20(23)25-17-12-15-18-13-9-8-10

InchiKey: JPBMFFPSKJVVCN-UHFFFAOYSA-N

Formula: C21H32O4

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

Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-226.65	kJ/mol	Joback Method
hf	-738.59	kJ/mol	Joback Method
hfus	42.35	kJ/mol	Joback Method
hvap	81.63	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.702		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1282.83	kPa	Joback Method
rinpol	2324.00		NIST Webbook
tb	855.91	K	Joback Method
tc	1060.47	K	Joback Method
tf	499.59	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.54	J/mol×K	855.91	Joback Method
cpg	955.09	J/mol×K	890.00	Joback Method
cpg	970.47	J/mol×K	924.10	Joback Method
cpg	984.71	J/mol×K	958.19	Joback Method
cpg	997.88	J/mol×K	992.28	Joback Method
cpg	1010.03	J/mol×K	1026.38	Joback Method
cpg	1021.19	J/mol×K	1060.47	Joback Method
dvisc	0.0005772	Pa×s	499.59	Joback Method
dvisc	0.0002862	Pa×s	558.98	Joback Method

dvisc	0.0001624	Pa×s	618.36	Joback Method
dvisc	0.0001018	Pa×s	677.75	Joback Method
dvisc	0.0000688	Pa×s	737.14	Joback Method
dvisc	0.0000493	Pa×s	796.52	Joback Method
dvisc	0.0000370	Pa×s	855.91	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=U361836&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