Dimethylmalonic acid, pentyl 3-phenylpropyl ester

Inchi: InChI=1S/C19H28O4/c1-4-5-9-14-22-17(20)19(2,3)18(21)23-15-10-13-16-11-7-6-8-12-16

InchiKey: XLSRUFAIYJHDEG-UHFFFAOYSA-N

Formula: C19H28O4

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

Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-243.49	kJ/mol	Joback Method
hf	-697.31	kJ/mol	Joback Method
hfus	37.17	kJ/mol	Joback Method
hvap	77.18	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.922		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
rinpol	2133.00		NIST Webbook
rinpol	2133.00		NIST Webbook
tb	810.15	K	Joback Method
tc	1014.93	K	Joback Method
tf	477.05	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.04	J/mol×K	810.15	Joback Method
cpg	891.24	J/mol×K	980.80	Joback Method
cpg	879.29	J/mol×K	946.67	Joback Method
cpg	866.33	J/mol×K	912.54	Joback Method
cpg	852.34	J/mol×K	878.41	Joback Method
cpg	837.26	J/mol×K	844.28	Joback Method
cpg	902.23	J/mol×K	1014.93	Joback Method
dvisc	0.0000498	Pa×s	810.15	Joback Method

dvisc	0.0000661	Pa×s	754.63	Joback Method
dvisc	0.0000917	Pa×s	699.12	Joback Method
dvisc	0.0001346	Pa×s	643.60	Joback Method
dvisc	0.0002124	Pa×s	588.08	Joback Method
dvisc	0.0003686	Pa×s	532.57	Joback Method
dvisc	0.0007273	Pa×s	477.05	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=U361833&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