Dimethylmalonic acid, isohexyl 2-phenethyl ester

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

InchiKey: AENCDLIBAUVBGF-UHFFFAOYSA-N

Formula: C19H28O4

SMILES: CC(C)CCCOC(=O)C(C)(C)C(=O)OCCc1ccccc1

Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-245.93	kJ/mol	Joback Method
hf	-702.59	kJ/mol	Joback Method
hfus	33.64	kJ/mol	Joback Method
hvap	76.79	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.778		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	2078.00		NIST Webbook
tb	809.71	K	Joback Method
tc	1016.99	K	Joback Method
tf	462.05	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.57	J/mol×K	809.71	Joback Method
cpg	892.36	J/mol×K	982.44	Joback Method
cpg	880.36	J/mol×K	947.89	Joback Method
cpg	867.33	J/mol×K	913.35	Joback Method
cpg	853.22	J/mol×K	878.80	Joback Method
cpg	837.98	J/mol×K	844.26	Joback Method
cpg	903.37	J/mol×K	1016.99	Joback Method
dvisc	0.0000458	Pa×s	809.71	Joback Method
dvisc	0.0000618	Pa×s	751.77	Joback Method

dvisc	0.0000876	Pa×s	693.82	Joback Method
dvisc	0.0001325	Pa×s	635.88	Joback Method
dvisc	0.0002176	Pa×s	577.94	Joback Method
dvisc	0.0003993	Pa×s	519.99	Joback Method
dvisc	0.0008531	Pa×s	462.05	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U361618&Units=SI

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