Dimethylmalonic acid, heptyl 3-methylphenyl ester

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

InchiKey: DGBOTRJUYMCQLN-UHFFFAOYSA-N

Formula: C19H28O4

SMILES: CCCCCCCOC(=O)C(C)(C)C(=O)Oc1cccc(C)c1

Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-253.12	kJ/mol	Joback Method
hf	-708.78	kJ/mol	Joback Method
hfus	36.78	kJ/mol	Joback Method
hvap	77.84	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.440		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1462.37	kPa	Joback Method
rinpol	2108.00		NIST Webbook
tb	815.13	K	Joback Method
tc	1020.72	K	Joback Method
tf	489.57	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.35	J/mol×K	815.13	Joback Method
cpg	836.47	J/mol×K	849.40	Joback Method
cpg	851.47	J/mol×K	883.66	Joback Method
cpg	865.37	J/mol×K	917.93	Joback Method
cpg	878.23	J/mol×K	952.19	Joback Method
cpg	890.08	J/mol×K	986.46	Joback Method
cpg	900.96	J/mol×K	1020.72	Joback Method
dvisc	0.0006091	Pa×s	489.57	Joback Method
dvisc	0.0003266	Pa×s	543.83	Joback Method

dvisc	0.0001960	Pa×s	598.09	Joback Method
dvisc	0.0001281	Pa×s	652.35	Joback Method
dvisc	0.0000894	Pa×s	706.61	Joback Method
dvisc	0.0000656	Pa×s	760.87	Joback Method
dvisc	0.0000502	Pa×s	815.13	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=U363615&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