Dimethylmalonic acid, di(trans-4-methylcyclohexyl) ester

Inchi: InChI=1S/C19H32O4/c1-13-5-9-15(10-6-13)22-17(20)19(3,4)18(21)23-16-11-7-14(2)8-12

InchiKey: ZVDVSVAEMPCQCL-UHFFFAOYSA-N

Formula: C19H32O4

SMILES: CC1CCC(OC(=O)C(C)(C)C(=O)OC2CCC(C)CC2)CC1

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-322.42	kJ/mol	Joback Method
hf	-865.88	kJ/mol	Joback Method
hfus	28.94	kJ/mol	Joback Method
hvap	75.14	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.256		Crippen Method
mcvol	271.730	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	2109.00		NIST Webbook
rinpol	2109.00		NIST Webbook
tb	813.23	K	Joback Method
tc	1037.22	K	Joback Method
tf	456.91	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.85	J/mol×K	813.23	Joback Method
cpg	931.39	J/mol×K	850.56	Joback Method
cpg	951.09	J/mol×K	887.89	Joback Method
cpg	968.98	J/mol×K	925.23	Joback Method
cpg	985.10	J/mol×K	962.56	Joback Method
cpg	999.49	J/mol×K	999.89	Joback Method
cpg	1012.19	J/mol×K	1037.22	Joback Method
dvisc	0.0012971	Pa×s	456.91	Joback Method

dvisc	0.0006362	Pa×s	516.30	Joback Method
dvisc	0.0003614	Pa×s	575.68	Joback Method
dvisc	0.0002283	Pa×s	635.07	Joback Method
dvisc	0.0001559	Pa×s	694.46	Joback Method
dvisc	0.0001131	Pa×s	753.84	Joback Method
dvisc	0.0000860	Pa×s	813.23	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=U363904&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