Diethylmalonic acid, 2,6-dimethoxyphenyl isobutyl ester

Inchi: InChI=1S/C19H28O6/c1-7-19(8-2,17(20)24-12-13(3)4)18(21)25-16-14(22-5)10-9-11-15(1

InchiKey: ZUOGJRNTNSGRAM-UHFFFAOYSA-N

Formula: C19H28O6

SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 352.42

Physical Properties

Property code	Value	Unit	Source
gf	-475.19	kJ/mol	Joback Method
hf	-989.97	kJ/mol	Joback Method
hfus	35.24	kJ/mol	Joback Method
hvap	82.94	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.615		Crippen Method
mcvol	281.430	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	2268.00		NIST Webbook
tb	864.51	K	Joback Method
tc	1073.56	K	Joback Method
tf	531.55	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.67	J/mol×K	864.51	Joback Method
cpg	940.09	J/mol×K	1038.72	Joback Method
cpg	930.18	J/mol×K	1003.88	Joback Method
cpg	918.98	J/mol×K	969.04	Joback Method
cpg	906.50	J/mol×K	934.19	Joback Method
cpg	892.73	J/mol×K	899.35	Joback Method
cpg	948.74	J/mol×K	1073.56	Joback Method
dvisc	0.0000259	Pa×s	864.51	Joback Method
dvisc	0.0000336	Pa×s	809.02	Joback Method

dvisc	0.0000453	Pa×s	753.52	Joback Method
dvisc	0.0000641	Pa×s	698.03	Joback Method
dvisc	0.0000962	Pa×s	642.54	Joback Method
dvisc	0.0001562	Pa×s	587.04	Joback Method
dvisc	0.0002803	Pa×s	531.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369811&Units=SI
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

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