Diethylmalonic acid, di(3-methoxyphenyl) ester

Inchi: InChI=1S/C21H24O6/c1-5-21(6-2,19(22)26-17-11-7-9-15(13-17)24-3)20(23)27-18-12-8-1

InchiKey: JYGDUBSIFOBSOT-UHFFFAOYSA-N

Formula: C21H24O6

SMILES: CCC(CC)(C(=O)Oc1cccc(OC)c1)C(=O)Oc1cccc(OC)c1

Mol. weight [g/mol]: 372.41

Physical Properties

Property code	Value	Unit	Source
gf	-343.50	kJ/mol	Joback Method
hf	-789.44	kJ/mol	Joback Method
hfus	37.99	kJ/mol	Joback Method
hvap	90.05	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.021		Crippen Method
mcvol	285.850	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
rinpol	2668.00		NIST Webbook
rinpol	2668.00		NIST Webbook
tb	937.39	K	Joback Method
tc	1166.72	K	Joback Method
tf	595.51	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.05	J/mol×K	937.39	Joback Method
cpg	905.78	J/mol×K	975.61	Joback Method
cpg	917.00	J/mol×K	1013.83	Joback Method
cpg	926.72	J/mol×K	1052.05	Joback Method
cpg	934.98	J/mol×K	1090.27	Joback Method
cpg	941.79	J/mol×K	1128.50	Joback Method
cpg	947.19	J/mol×K	1166.72	Joback Method
dvisc	0.0001790	Pa×s	595.51	Joback Method

dvisc	0.0001075	Pa×s	652.49	Joback Method
dvisc	0.0000701	Pa×s	709.47	Joback Method
dvisc	0.0000487	Pa×s	766.45	Joback Method
dvisc	0.0000356	Pa×s	823.43	Joback Method
dvisc	0.0000271	Pa×s	880.41	Joback Method
dvisc	0.0000213	Pa×s	937.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370877&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

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