Diethylmalonic acid, 3-methoxyphenyl pentyl ester

Inchi: InChI=1S/C19H28O5/c1-5-8-9-13-23-17(20)19(6-2,7-3)18(21)24-16-12-10-11-15(14-16)2

InchiKey: NTPBVLFVIJLLMU-UHFFFAOYSA-N

Formula: C19H28O5

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

Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-358.12	kJ/mol	Joback Method
hf	-841.00	kJ/mol	Joback Method
hfus	37.97	kJ/mol	Joback Method
hvap	80.25	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.140		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinpol	2231.00		NIST Webbook
rinpol	2231.00		NIST Webbook
tb	837.55	K	Joback Method
tc	1043.24	K	Joback Method
tf	511.80	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.26	J/mol×K	837.55	Joback Method
cpg	864.87	J/mol×K	871.83	Joback Method
cpg	879.30	J/mol×K	906.11	Joback Method
cpg	892.58	J/mol×K	940.40	Joback Method
cpg	904.73	J/mol×K	974.68	Joback Method
cpg	915.78	J/mol×K	1008.96	Joback Method
cpg	925.75	J/mol×K	1043.24	Joback Method
dvisc	0.0004207	Pa×s	511.80	Joback Method

dvisc	0.0002318	Pa×s	566.09	Joback Method
dvisc	0.0001418	Pa×s	620.38	Joback Method
dvisc	0.0000938	Pa×s	674.67	Joback Method
dvisc	0.0000660	Pa×s	728.97	Joback Method
dvisc	0.0000488	Pa×s	783.26	Joback Method
dvisc	0.0000375	Pa×s	837.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370872&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