Diethylmalonic acid, 3-methoxyphenyl propyl ester

Inchi: InChI=1S/C17H24O5/c1-5-11-21-15(18)17(6-2,7-3)16(19)22-14-10-8-9-13(12-14)20-4/h8
InchiKey: VRJIJRMCYRNKQN-UHFFFAOYSA-N
Formula: C17H24O5
SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(OC)c1
Mol. weight [g/mol]: 308.37

Physical Properties

Property code	Value	Unit	Source
gf	-374.96	kJ/mol	Joback Method
hf	-799.72	kJ/mol	Joback Method
hfus	32.79	kJ/mol	Joback Method
hvap	75.80	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.360		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpol	2072.00		NIST Webbook
tb	791.79	K	Joback Method
tc	999.14	K	Joback Method
tf	489.26	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.33	J/mol×K	791.79	Joback Method
cpg	749.58	J/mol×K	826.35	Joback Method
cpg	763.73	J/mol×K	860.91	Joback Method
cpg	776.78	J/mol×K	895.47	Joback Method
cpg	788.76	J/mol×K	930.02	Joback Method
cpg	799.68	J/mol×K	964.58	Joback Method
cpg	809.58	J/mol×K	999.14	Joback Method
dvisc	0.0005202	Pa×s	489.26	Joback Method
dvisc	0.0002938	Pa×s	539.68	Joback Method

dvisc	0.0001829	Pa×s	590.10	Joback Method
dvisc	0.0001227	Pa×s	640.52	Joback Method
dvisc	0.0000873	Pa×s	690.95	Joback Method
dvisc	0.0000650	Pa×s	741.37	Joback Method
dvisc	0.0000503	Pa×s	791.79	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U370869&Units=SI

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