Diethylmalonic acid, ethyl 3-phenylpropyl ester

Inchi: InChI=1S/C18H26O4/c1-4-18(5-2,16(19)21-6-3)17(20)22-14-10-13-15-11-8-7-9-12-15/h7

InchiKey: POMWAAUAKUJFNG-UHFFFAOYSA-N

Formula: C18H26O4

SMILES: CCOC(=O)C(CC)(CC)C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-251.91	kJ/mol	Joback Method
hf	-676.67	kJ/mol	Joback Method
hfus	34.58	kJ/mol	Joback Method
hvap	74.95	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.532		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2041.00		NIST Webbook
rinpol	2041.00		NIST Webbook
tb	787.27	K	Joback Method
tc	993.13	K	Joback Method
tf	465.78	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.54	J/mol×K	787.27	Joback Method
cpg	832.99	J/mol×K	958.82	Joback Method
cpg	821.17	J/mol×K	924.51	Joback Method
cpg	808.35	J/mol×K	890.20	Joback Method
cpg	794.50	J/mol×K	855.89	Joback Method
cpg	779.58	J/mol×K	821.58	Joback Method
cpg	843.88	J/mol×K	993.13	Joback Method
dvisc	0.0000577	Pa×s	787.27	Joback Method

dvisc	0.0000763	Pa×s	733.69	Joback Method
dvisc	0.0001055	Pa×s	680.11	Joback Method
dvisc	0.0001542	Pa×s	626.52	Joback Method
dvisc	0.0002418	Pa×s	572.94	Joback Method
dvisc	0.0004162	Pa×s	519.36	Joback Method
dvisc	0.0008118	Pa×s	465.78	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=U369650&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