Diethylmalonic acid, heptyl isopropyl ester

Inchi: InChI=1S/C17H32O4/c1-6-9-10-11-12-13-20-15(18)17(7-2,8-3)16(19)21-14(4)5/h14H,6-1
InchiKey: YBWAXVWXNJQBOH-UHFFFAOYSA-N
Formula: C17H32O4
SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)C
Mol. weight [g/mol]: 300.43

Physical Properties

Property code	Value	Unit	Source
gf	-375.18	kJ/mol	Joback Method
hf	-897.84	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	70.06	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.258		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	1733.00		NIST Webbook
rinpol	1733.00		NIST Webbook
tb	737.27	K	Joback Method
tc	921.13	K	Joback Method
tf	413.09	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.34	J/mol×K	737.27	Joback Method
cpg	810.75	J/mol×K	767.91	Joback Method
cpg	827.21	J/mol×K	798.56	Joback Method
cpg	842.74	J/mol×K	829.20	Joback Method
cpg	857.37	J/mol×K	859.84	Joback Method
cpg	871.12	J/mol×K	890.49	Joback Method
cpg	884.02	J/mol×K	921.13	Joback Method
dvisc	0.0013901	Pa×s	413.09	Joback Method

dvisc	0.0006127	Pa×s	467.12	Joback Method
dvisc	0.0003200	Pa×s	521.15	Joback Method
dvisc	0.0001889	Pa×s	575.18	Joback Method
dvisc	0.0001220	Pa×s	629.21	Joback Method
dvisc	0.0000845	Pa×s	683.24	Joback Method
dvisc	0.0000617	Pa×s	737.27	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=U370267&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