Diethylmalonic acid, pentyl tetrahydrofurfuryl ester

Inchi: InChI=1S/C17H30O5/c1-4-7-8-11-21-15(18)17(5-2,6-3)16(19)22-13-14-10-9-12-20-14/h1

InchiKey: IMLKFDBVHWPKQR-UHFFFAOYSA-N

Formula: C17H30O5

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)OCC1CCCO1

Mol. weight [g/mol]: 314.42

Physical Properties

Property code	Value	Unit	Source
gf	-422.31	kJ/mol	Joback Method
hf	-964.08	kJ/mol	Joback Method
hfus	39.86	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.248		Crippen Method
mcvol	260.280	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	1971.00		NIST Webbook
tb	779.94	K	Joback Method
tc	978.20	K	Joback Method
tf	465.56	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.34	J/mol×K	779.94	Joback Method
cpg	836.87	J/mol×K	812.98	Joback Method
cpg	853.27	J/mol×K	846.03	Joback Method
cpg	868.56	J/mol×K	879.07	Joback Method
cpg	882.79	J/mol×K	912.12	Joback Method
cpg	895.98	J/mol×K	945.16	Joback Method
cpg	908.18	J/mol×K	978.20	Joback Method
dvisc	0.0011563	Pa×s	465.56	Joback Method
dvisc	0.0005991	Pa×s	517.96	Joback Method

dvisc	0.0003503	Pa×s	570.35	Joback Method
dvisc	0.0002242	Pa×s	622.75	Joback Method
dvisc	0.0001537	Pa×s	675.15	Joback Method
dvisc	0.0001113	Pa×s	727.54	Joback Method
dvisc	0.0000842	Pa×s	779.94	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=U370640&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