2,4-Hexadienedioic acid, diethyl ester

Other names: Diethyl 2,4-hexadienedioate
Inchi: InChI=1S/C10H14O4/c1-3-13-9(11)7-5-6-8-10(12)14-4-2/h5-8H,3-4H2,1-2H3/b7-5+,8-6+
InchiKey: VHIYCPCXACHVJM-KQQUZDAGSA-N
Formula: C10H14O4
SMILES: CCOC(=O)C=CC=CC(=O)OCC
Mol. weight [g/mol]: 198.22
CAS: 1441-57-2

Physical Properties

Property code	Value	Unit	Source
gf	-274.08	kJ/mol	Joback Method
hf	-504.89	kJ/mol	Joback Method
hfus	27.63	kJ/mol	Joback Method
hvap	56.08	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.225		Crippen Method
mcvol	158.040	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1380.00		NIST Webbook
tb	589.10	K	Joback Method
tc	783.77	K	Joback Method
tf	336.62	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.82	J/mol×K	589.10	Joback Method
cpg	387.99	J/mol×K	621.54	Joback Method
cpg	399.55	J/mol×K	653.99	Joback Method
cpg	410.53	J/mol×K	686.43	Joback Method
cpg	420.92	J/mol×K	718.88	Joback Method
cpg	430.75	J/mol×K	751.32	Joback Method
cpg	440.04	J/mol×K	783.77	Joback Method

dvisc	0.0016250	Pa×s	336.62	Joback Method
dvisc	0.0008562	Pa×s	378.70	Joback Method
dvisc	0.0005128	Pa×s	420.78	Joback Method
dvisc	0.0003372	Pa×s	462.86	Joback Method
dvisc	0.0002377	Pa×s	504.94	Joback Method
dvisc	0.0001769	Pa×s	547.02	Joback Method
dvisc	0.0001373	Pa×s	589.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1441572&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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