2,4-Hexadienoic acid, methyl ester

Other names: Methyl 2,4-hexadienoate
methyl hexa-2,4-dienoate
Inchi: InChI=1S/C7H10O2/c1-3-4-5-6-7(8)9-2/h3-6H,1-2H3
InchiKey: KWKVAGQCDSHWFK-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CC=CC=CC(=O)OC
Mol. weight [g/mol]: 126.15
CAS: 1515-80-6

Physical Properties

Property code	Value	Unit	Source
gf	-65.42	kJ/mol	Joback Method
hf	-198.17	kJ/mol	Joback Method
hfus	17.08	kJ/mol	Joback Method
hvap	40.25	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.292		Crippen Method
mcvol	108.330	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	1021.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	991.00		NIST Webbook
ripol	1444.00		NIST Webbook
tb	444.17	K	Joback Method
tc	638.38	K	Joback Method
tf	230.65	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.48	J/mol×K	444.17	Joback Method
cpg	216.82	J/mol×K	476.54	Joback Method
cpg	226.65	J/mol×K	508.91	Joback Method
cpg	235.98	J/mol×K	541.28	Joback Method
cpg	244.83	J/mol×K	573.65	Joback Method
cpg	253.23	J/mol×K	606.02	Joback Method
cpg	261.19	J/mol×K	638.38	Joback Method
dvisc	0.0027062	Pa×s	230.65	Joback Method
dvisc	0.0012812	Pa×s	266.24	Joback Method
dvisc	0.0007235	Pa×s	301.82	Joback Method
dvisc	0.0004609	Pa×s	337.41	Joback Method
dvisc	0.0003200	Pa×s	373.00	Joback Method
dvisc	0.0002368	Pa×s	408.58	Joback Method
dvisc	0.0001838	Pa×s	444.17	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	349.00 ± 1.00	K	2.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1515806&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume