2,4-Heptadienoic acid, 6-methyl-, ethyl ester

Inchi: InChI=1S/C10H16O2/c1-4-12-10(11)8-6-5-7-9(2)3/h5-9H,4H2,1-3H3/b7-5+,8-6+
InchiKey: SFUYOPHWNDIHFL-KQQUZDAGSA-N
Formula: C10H16O2
SMILES: CCOC(=O)C=CC=CC(C)C
Mol. weight [g/mol]: 168.23
CAS: 10236-06-3

Physical Properties

Property code	Value	Unit	Source
gf	-42.60	kJ/mol	Joback Method
hf	-265.37	kJ/mol	Joback Method
hfus	21.32	kJ/mol	Joback Method
hvap	46.54	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.318		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1296.00		NIST Webbook
rinpol	1296.00		NIST Webbook
tb	512.37	K	Joback Method
tc	704.09	K	Joback Method
tf	249.46	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.37	J/mol×K	512.37	Joback Method
cpg	395.69	J/mol×K	672.14	Joback Method
cpg	384.49	J/mol×K	640.18	Joback Method
cpg	372.69	J/mol×K	608.23	Joback Method
cpg	360.25	J/mol×K	576.28	Joback Method
cpg	347.15	J/mol×K	544.32	Joback Method
cpg	406.32	J/mol×K	704.09	Joback Method

dvisc	0.0001498	Pa×s	512.37	Joback Method
dvisc	0.0002010	Pa×s	468.55	Joback Method
dvisc	0.0002866	Pa×s	424.73	Joback Method
dvisc	0.0004433	Pa×s	380.91	Joback Method
dvisc	0.0007680	Pa×s	337.10	Joback Method
dvisc	0.0015682	Pa×s	293.28	Joback Method
dvisc	0.0041146	Pa×s	249.46	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10236063&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume