Ethyl 4,7-octadienoate

Inchi: InChI=1S/C10H16O2/c1-3-5-6-7-8-9-10(11)12-4-2/h3,6-7H,1,4-5,8-9H2,2H3/b7-6+
InchiKey: LNOWXPKCCJROHI-VOTSOKGWSA-N
Formula: C10H16O2
SMILES: C=CC/C=C/CCC(=O)OCC
Mol. weight [g/mol]: 168.24

Physical Properties

Property code	Value	Unit	Source
af	0.4082		Cheméo Relay (1.0)
gf	-32.54	kJ/mol	Joback Method
hf	-367.87	kJ/mol	Cheméo Relay (1.0)
hfus	23.36	kJ/mol	Joback Method
hvap	59.71	kJ/mol	Cheméo Relay (1.0)
ie	8.97	eV	Cheméo Relay (1.0)
log10ws	-2.45		Cheméo Relay (1.0)
logp	2.462		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
tb	463.68	K	Cheméo Relay (1.0)
tc	654.88	K	Cheméo Relay (1.0)
tf	211.77	K	Cheméo Relay (1.0)
vc	0.524	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.46	J/mol×K	505.33	Joback Method
cpg	403.24	J/mol×K	688.59	Joback Method
cpg	392.82	J/mol×K	658.05	Joback Method
cpg	381.88	J/mol×K	627.50	Joback Method
cpg	370.39	J/mol×K	596.96	Joback Method
cpg	358.33	J/mol×K	566.42	Joback Method
cpg	345.70	J/mol×K	535.87	Joback Method
dvisc	0.0004852	Pa×s	386.55	Joback Method

dvisc	0.0001912	Pa×s	505.33	Joback Method
dvisc	0.0002474	Pa×s	465.74	Joback Method
dvisc	0.0003358	Pa×s	426.15	Joback Method
dvisc	0.0028123	Pa×s	267.78	Joback Method
dvisc	0.0007625	Pa×s	346.96	Joback Method
dvisc	0.0013463	Pa×s	307.37	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72276096&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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