TRANS-2-HEPTENYL ACETATE

Other names: 2-Hepten-1-ol, acetate, (E)-
(2E)-2-Heptenyl acetate
(E)-2-Heptenyl acetate
(E)-hept-2-enyl acetate
Inchi: InChI=1S/C9H16O2/c1-3-4-5-6-7-8-11-9(2)10/h6-7H,3-5,8H2,1-2H3/b7-6+
InchiKey: AWCPMVVOGVEPRC-VOTSOKGWSA-N
Formula: C9H16O2
SMILES: CCCC/C=C/COC(C)=O
Mol. weight [g/mol]: 156.23

Physical Properties

Property code	Value	Unit	Source
af	0.4499		Cheméo Relay (1.0)
gf	-128.80	kJ/mol	Joback Method
hf	-445.43	kJ/mol	Cheméo Relay (1.0)
hfus	22.06	kJ/mol	Joback Method
hvap	55.17	kJ/mol	Cheméo Relay (1.0)
ie	9.10	eV	Cheméo Relay (1.0)
log10ws	-2.81		Cheméo Relay (1.0)
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
ripol	1427.00		NIST Webbook
ripol	1427.00		NIST Webbook
tb	454.89	K	Cheméo Relay (1.0)
tc	631.02	K	Cheméo Relay (1.0)
tf	193.58	K	Cheméo Relay (1.0)
vc	0.514	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.02	J/mol×K	485.77	Joback Method
cpg	318.93	J/mol×K	516.03	Joback Method

cpg	331.30	J/mol×K	546.29	Joback Method
cpg	343.15	J/mol×K	576.54	Joback Method
cpg	354.47	J/mol×K	606.80	Joback Method
cpg	365.29	J/mol×K	637.06	Joback Method
cpg	375.62	J/mol×K	667.32	Joback Method
dvisc	0.0030655	Pa×s	258.27	Joback Method
dvisc	0.0014558	Pa×s	296.19	Joback Method
dvisc	0.0008186	Pa×s	334.10	Joback Method
dvisc	0.0005177	Pa×s	372.02	Joback Method
dvisc	0.0003563	Pa×s	409.94	Joback Method
dvisc	0.0002612	Pa×s	447.85	Joback Method
dvisc	0.0002011	Pa×s	485.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16939734&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

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
ripol:	Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume