(E,Z)-2,4-heptadienal

Inchi: InChI=1S/C7H10O/c1-2-3-4-5-6-7-8/h3-7H,2H2,1H3/b4-3+,6-5+
InchiKey: SATICYYAWWYRAM-VNKDHWASSA-N
Formula: C7H10O
SMILES: CC/C=C\C=C\C=O
Mol. weight [g/mol]: 110.16

Physical Properties

Property code	Value	Unit	Source
af	0.3024		Cheméo Relay (1.0)
gf	68.98	kJ/mol	Joback Method
hf	-86.16	kJ/mol	Cheméo Relay (1.0)
hfus	16.58	kJ/mol	Joback Method
hvap	48.15	kJ/mol	Cheméo Relay (1.0)
ie	9.00	eV	Cheméo Relay (1.0)
logp	1.708		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	428.32	K	Cheméo Relay (1.0)
tc	628.77	K	Cheméo Relay (1.0)
tf	244.05	K	Cheméo Relay (1.0)
vc	0.359	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.30	J/mol×K	416.54	Joback Method
cpg	240.28	J/mol×K	606.14	Joback Method
cpg	232.55	J/mol×K	574.54	Joback Method
cpg	224.36	J/mol×K	542.94	Joback Method
cpg	215.67	J/mol×K	511.34	Joback Method
cpg	206.45	J/mol×K	479.74	Joback Method
cpg	196.67	J/mol×K	448.14	Joback Method
dvisc	0.0005608	Pa×s	308.51	Joback Method
dvisc	0.0002197	Pa×s	416.54	Joback Method

dvisc	0.0002831	Pa×s	380.53	Joback Method
dvisc	0.0003844	Pa×s	344.52	Joback Method
dvisc	0.0039290	Pa×s	200.49	Joback Method
dvisc	0.0009040	Pa×s	272.51	Joback Method
dvisc	0.0016852	Pa×s	236.50	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4313024&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):

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
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