E-9-TETRADECENAL

Other names: 9-tetradecenal, E
Inchi: InChI=1S/C14H26O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15/h5-6,14H,2-4,7-13H2,1H3/b6-
InchiKey: ANJAOCICJSRZSR-AATRIKPKSA-N
Formula: C14H26O
SMILES: CCCC/C=C/CCCCCCCC=O
Mol. weight [g/mol]: 210.36

Physical Properties

Property code	Value	Unit	Source
af	0.6414		Cheméo Relay (1.0)
gf	47.70	kJ/mol	Joback Method
hf	-342.89	kJ/mol	Cheméo Relay (1.0)
hfus	34.51	kJ/mol	Joback Method
hvap	77.42	kJ/mol	Cheméo Relay (1.0)
ie	8.90	eV	Cheméo Relay (1.0)
log10ws	-5.22		Cheméo Relay (1.0)
logp	4.662		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	1604.00		NIST Webbook
rinpol	1604.00		NIST Webbook
ripol	1942.00		NIST Webbook
ripol	1942.00		NIST Webbook
tb	543.09	K	Cheméo Relay (1.0)
tc	731.31	K	Cheméo Relay (1.0)
tf	274.20	K	Cheméo Relay (1.0)
vc	0.764	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.54	J/mol×K	572.54	Joback Method
cpg	535.03	J/mol×K	601.00	Joback Method
cpg	550.80	J/mol×K	629.46	Joback Method

cpg	565.86	J/mol×K	657.91	Joback Method
cpg	580.24	J/mol×K	686.37	Joback Method
cpg	593.97	J/mol×K	714.83	Joback Method
cpg	607.07	J/mol×K	743.29	Joback Method
dvisc	0.0043394	Pa×s	284.46	Joback Method
dvisc	0.0017423	Pa×s	332.47	Joback Method
dvisc	0.0008807	Pa×s	380.49	Joback Method
dvisc	0.0005187	Pa×s	428.50	Joback Method
dvisc	0.0003399	Pa×s	476.51	Joback Method
dvisc	0.0002406	Pa×s	524.53	Joback Method
dvisc	0.0001805	Pa×s	572.54	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U131357&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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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