3-tetradecenal, Z

Other names: (Z)-3-Tetradecenal
Inchi: InChI=1S/C14H26O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15/h11-12,14H,2-10,13H2,1H3/b
InchiKey: FXDAKNIBIGFIJX-QXMHVHEDSA-N
Formula: C14H26O
SMILES: CCCCCCCCCCC=CCC=O
Mol. weight [g/mol]: 210.36

Physical Properties

Property code	Value	Unit	Source
gf	47.70	kJ/mol	Joback Method
hf	-300.65	kJ/mol	Joback Method
hfus	34.51	kJ/mol	Joback Method
hvap	53.44	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.662		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	1599.00		NIST Webbook
rinpol	1599.00		NIST Webbook
ripol	1945.00		NIST Webbook
ripol	1945.00		NIST Webbook
tb	572.54	K	Joback Method
tc	743.29	K	Joback Method
tf	284.46	K	Joback Method
vc	0.817	m3/kmol	Joback Method

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=R265555&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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