

4-tetradecenal, E

Inchi:	InChI=1S/C14H26O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15/h10-11,14H,2-9,12-13H2,1H3
InchiKey:	MRSXTPSFUFLUIT-ZHACJKMWSA-N
Formula:	C14H26O
SMILES:	CCCCCCCCC=CCCC=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	1602.00		NIST Webbook
rinpol	1602.00		NIST Webbook
ripol	1940.00		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/molxK	572.54	Joback Method
cpg	593.97	J/molxK	714.83	Joback Method
cpg	580.24	J/molxK	686.37	Joback Method
cpg	565.86	J/molxK	657.91	Joback Method
cpg	550.80	J/molxK	629.46	Joback Method
cpg	535.03	J/molxK	601.00	Joback Method
cpg	607.07	J/molxK	743.29	Joback Method

dvisc	0.0001805	Paxs	572.54	Joback Method
dvisc	0.0002406	Paxs	524.53	Joback Method
dvisc	0.0003399	Paxs	476.51	Joback Method
dvisc	0.0005187	Paxs	428.50	Joback Method
dvisc	0.0008807	Paxs	380.49	Joback Method
dvisc	0.0017423	Paxs	332.47	Joback Method
dvisc	0.0043394	Paxs	284.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R275740&Units=SI

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
mvol:	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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