

(Z)-2-PentylNon-2-enal

Inchi:	InChI=1S/C14H26O/c1-3-5-7-8-10-12-14(13-15)11-9-6-4-2/h12-13H,3-11H2,1-2H3/b14-1
InchiKey:	VIKQYIINCNAGJW-OWBHPGMISA-N
Formula:	C14H26O
SMILES:	CCCCCCC=C(C=O)CCCC
Mol. weight [g/mol]:	210.36

Physical Properties

Property code	Value	Unit	Source
gf	39.15	kJ/mol	Joback Method
hf	-310.44	kJ/mol	Joback Method
hfus	33.20	kJ/mol	Joback Method
hvap	53.52	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.662		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
ripol	1884.00		NIST Webbook
ripol	1884.00		NIST Webbook
tb	572.42	K	Joback Method
tc	745.67	K	Joback Method
tf	270.50	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.31	J/molxK	572.42	Joback Method
cpg	535.02	J/molxK	601.30	Joback Method
cpg	550.98	J/molxK	630.17	Joback Method
cpg	566.21	J/molxK	659.05	Joback Method
cpg	580.75	J/molxK	687.92	Joback Method
cpg	594.62	J/molxK	716.80	Joback Method

Sources

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=R341961&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	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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