(E)-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-WYMLVPIESA-N
Formula: C14H26O
SMILES: CCCCCCC=C(C=O)CCCCC
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	1570.00		NIST Webbook
rinpol	1570.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1900.00		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/mol×K	572.42	Joback Method
cpg	535.02	J/mol×K	601.30	Joback Method
cpg	550.98	J/mol×K	630.17	Joback Method
cpg	566.21	J/mol×K	659.05	Joback Method
cpg	580.75	J/mol×K	687.92	Joback Method
cpg	594.62	J/mol×K	716.80	Joback Method

cpg	607.86	J/mol×K	745.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R341916&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
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