9-Undecenal, 2,6,10-trimethyl-

Other names:	2,6,10-Trimethyl-9-undecen-1-al
	2,6,10-Trimethyl-9-undecenal
	2,6,10-trimethylundec-9-enal
	Adoxal
Inchi:	InChI=1S/C14H26O/c1-12(2)7-5-8-13(3)9-6-10-14(4)11-15/h7,11,13-14H,5-6,8-10H2,1-4
InchiKey:	UEGBWDUVDAKUGA-UHFFFAOYSA-N
Formula:	C14H26O
SMILES:	CC(C)=CCCC(C)CCCC(C)C=O
Mol. weight [g/mol]:	210.36
CAS:	141-13-9

Physical Properties

Property code	Value	Unit	Source
gf	34.27	kJ/mol	Joback Method
hf	-321.00	kJ/mol	Joback Method
hfus	26.15	kJ/mol	Joback Method
hvap	52.74	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.374		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	1387.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1387.00		NIST Webbook
tb	571.54	K	Joback Method
tc	751.07	K	Joback Method
tf	240.50	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.92	J/mol×K	571.54	Joback Method
cpg	536.34	J/mol×K	601.46	Joback Method

cpg	552.94	J/mol×K	631.38	Joback Method
cpg	568.75	J/mol×K	661.30	Joback Method
cpg	583.80	J/mol×K	691.23	Joback Method
cpg	598.13	J/mol×K	721.15	Joback Method
cpg	611.76	J/mol×K	751.07	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36509e+01
Coeff. B	-4.32368e+03
Coeff. C	-9.43700e+01
Temperature range (K), min.	417.92
Temperature range (K), max.	612.84

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141139&Units=SI

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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