

3-Tridecyne

Other names:	3-C13H24
	3-Tridecene
Inchi:	InChI=1S/C13H24/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-5,7,9-13H2,1-2H3
InchiKey:	HDLJOUCNTFYRPD-UHFFFAOYSA-N
Formula:	C13H24
SMILES:	CCC#CCCCCCCCCCC
Mol. weight [g/mol]:	180.33
CAS:	60186-78-9

Physical Properties

Property code	Value	Unit	Source
gf	261.38	kJ/mol	Joback Method
hf	-39.35	kJ/mol	Joback Method
hfus	32.55	kJ/mol	Joback Method
hvap	46.68	kJ/mol	Joback Method
ie	9.14 ± 0.03	eV	NIST Webbook
log10ws	-5.06		Crippen Method
logp	4.540		Crippen Method
mcvol	185.430	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	166.80		NIST Webbook
tb	505.84	K	Joback Method
tc	685.15	K	Joback Method
tf	342.37	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.07	J/mol×K	505.84	Joback Method
cpg	441.19	J/mol×K	535.72	Joback Method
cpg	457.61	J/mol×K	565.61	Joback Method
cpg	473.34	J/mol×K	595.49	Joback Method
cpg	488.41	J/mol×K	625.38	Joback Method

cpg	502.83	J/mol×K	655.26	Joback Method
cpg	516.62	J/mol×K	685.15	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58923e+01
Coeff. B	-4.76991e+03
Coeff. C	-8.32500e+01
Temperature range (K), min.	388.92
Temperature range (K), max.	534.05

Sources

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=C60186789&Units=SI
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/ci990307I

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
ie:	Ionization energy
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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