

2-Tridecyne

Other names:	2-C ₁₃ H ₂₄
Inchi:	InChI=1S/C13H24/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3,5,7-13H2,1-2H3
InchiKey:	ZGKKGWBQPYIOBH-UHFFFAOYSA-N
Formula:	C ₁₃ H ₂₄
SMILES:	CC#CCCCCCCCCCC
Mol. weight [g/mol]:	180.33
CAS:	28467-75-6

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	9.28 ± 0.02	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
ripol	1351.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1341.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1526.90		NIST Webbook
ripol	1549.90		NIST Webbook
ripol	1531.50		NIST Webbook
ripol	1552.90		NIST Webbook
tb	505.84	K	Joback Method
tc	685.15	K	Joback Method
tf	342.37	K	Joback Method
vc	0.726	m ³ /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	1.65985e+01
Coeff. B	-5.04535e+03
Coeff. C	-8.51960e+01
Temperature range (K), min.	394.52
Temperature range (K), max.	532.20

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C28467756&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/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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
hvac:	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
rinp:	Non-polar retention indices
rip:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/22-167-2/2-Tridecyne.pdf>

Generated by Cheméo on 2024-04-17 01:27:14.768141495 +0000 UTC m=+15606483.688718808.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.