

1-Tridecyne

Other names:	1-C13H24 tridec-1-yne
Inchi:	InChI=1S/C13H24/c1-3-5-7-9-11-13-12-10-8-6-4-2/h1H,4-13H2,2H3
InchiKey:	GZEDKDBFUBPZNG-UHFFFAOYSA-N
Formula:	C13H24
SMILES:	C#CCCCCCCCCCCC
Mol. weight [g/mol]:	180.33
CAS:	26186-02-7

Physical Properties

Property code	Value	Unit	Source
gf	281.65	kJ/mol	Joback Method
hf	-19.75	kJ/mol	Joback Method
hfus	32.40	kJ/mol	Joback Method
hvap	44.39	kJ/mol	Joback Method
ie	9.90 ± 0.02	eV	NIST Webbook
log10ws	-5.06		Crippen Method
logp	4.540		Crippen Method
mcvol	185.430	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1298.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1283.00		NIST Webbook
ripol	1532.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1503.80		NIST Webbook
ripol	1526.10		NIST Webbook
ripol	1506.70		NIST Webbook
ripol	1527.20		NIST Webbook
tb	486.96	K	Joback Method
tc	656.86	K	Joback Method
tf	274.00 ± 3.00	K	NIST Webbook

vc	0.726	m ³ /kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.98	J/mol×K	486.96	Joback Method
cpg	436.58	J/mol×K	515.28	Joback Method
cpg	452.49	J/mol×K	543.59	Joback Method
cpg	467.73	J/mol×K	571.91	Joback Method
cpg	482.33	J/mol×K	600.23	Joback Method
cpg	496.30	J/mol×K	628.54	Joback Method
cpg	509.68	J/mol×K	656.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.60	K	3.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55192e+01
Coeff. B	-4.62412e+03
Coeff. C	-8.21400e+01
Temperature range (K), min.	385.73
Temperature range (K), max.	535.14

Sources

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=C26186027&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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