4-Tridecyne

Other names:	3-Tridecyne
	4-C13H24
	Tridec-4-yne
Inchi:	InChI=1S/C13H24/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-7,9,11-13H2,1-2H3
InchiKey:	HKALLPVHYMSWLE-UHFFFAOYSA-N
Formula:	C13H24
SMILES:	CCCC#CCCCCCCCC
Mol. weight [g/mol]:	180.33
CAS:	60186-79-0

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	9.07 ± 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	1312.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1315.00		NIST Webbook
ripol	1475.80		NIST Webbook
ripol	1478.70		NIST Webbook
ripol	1498.50		NIST Webbook
ripol	1479.70		NIST Webbook
ripol	1495.30		NIST Webbook
ripol	1476.50		NIST Webbook

ripol	1487.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1486.00		NIST Webbook
ripol	1486.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1497.90		NIST Webbook
ripol	1498.50		NIST Webbook
ripol	1461.20		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1479.70		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(Pvp) = 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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60186790&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/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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume