

3-Tridecen-1-yne, (Z)-

Other names:	(Z)-3-tridecen-1-yne
Inchi:	InChI=1S/C13H22/c1-3-5-7-9-11-13-12-10-8-6-4-2/h1,5,7H,4,6,8-13H2,2H3/b7-5-
InchiKey:	DIJCALIAWJLDBT-ALCCZGGFSA-N
Formula:	C13H22
SMILES:	C#CC=CCCCCCCCC
Mol. weight [g/mol]:	178.31
CAS:	37981-62-7

Physical Properties

Property code	Value	Unit	Source
gf	361.87	kJ/mol	Joback Method
hf	97.47	kJ/mol	Joback Method
hfus	32.60	kJ/mol	Joback Method
hvap	44.35	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.316		Crippen Method
mcvol	181.130	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
ripol	1363.00		NIST Webbook
ripol	1363.00		NIST Webbook
tb	491.12	K	Joback Method
tc	668.55	K	Joback Method
tf	278.16	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.51	J/molxK	491.12	Joback Method
cpg	419.88	J/molxK	520.69	Joback Method
cpg	435.48	J/molxK	550.26	Joback Method
cpg	450.36	J/molxK	579.83	Joback Method
cpg	464.53	J/molxK	609.40	Joback Method
cpg	478.05	J/molxK	638.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37981627&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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