

1,12-Tridecadiene

Other names:	Tridecadiene-1,12
Inchi:	InChI=1S/C13H24/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-4H,1-2,5-13H2
InchiKey:	BPHFKBMQSYNGQ-UHFFFAOYSA-N
Formula:	C13H24
SMILES:	C=CCCCCCCCCCC=C
Mol. weight [g/mol]:	180.33
CAS:	21964-48-7

Physical Properties

Property code	Value	Unit	Source
gf	234.26	kJ/mol	Joback Method
hf	-60.79	kJ/mol	Joback Method
hfus	26.87	kJ/mol	Joback Method
hvap	43.19	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.869		Crippen Method
mcvol	185.430	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	1279.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1279.00		NIST Webbook
ripol	1494.00		NIST Webbook
ripol	1434.00		NIST Webbook
tb	490.20	K	Joback Method
tc	656.13	K	Joback Method
tf	232.75	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.52	J/molxK	490.20	Joback Method
cpg	494.74	J/molxK	628.47	Joback Method
cpg	480.79	J/molxK	600.82	Joback Method

cpg	466.22	J/molxK	573.16	Joback Method
cpg	450.99	J/molxK	545.51	Joback Method
cpg	435.10	J/molxK	517.85	Joback Method
cpg	508.10	J/molxK	656.13	Joback Method
dvisc	0.0002044	Paxs	490.20	Joback Method
dvisc	0.0002690	Paxs	447.29	Joback Method
dvisc	0.0003753	Paxs	404.38	Joback Method
dvisc	0.0005668	Paxs	361.48	Joback Method
dvisc	0.0009564	Paxs	318.57	Joback Method
dvisc	0.0018994	Paxs	275.66	Joback Method
dvisc	0.0048581	Paxs	232.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21964487&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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

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