

Dodecane, 3-methyl-

Other names:	3-Methyldodecane
Inchi:	InChI=1S/C13H28/c1-4-6-7-8-9-10-11-12-13(3)5-2/h13H,4-12H2,1-3H3
InchiKey:	GRJUENNHVNYCHD-UHFFFAOYSA-N
Formula:	C13H28
SMILES:	CCCCCCCCC(C)CC
Mol. weight [g/mol]:	184.36
CAS:	17312-57-1

Physical Properties

Property code	Value	Unit	Source
gf	56.14	kJ/mol	Joback Method
hf	-316.93	kJ/mol	Joback Method
hfus	25.90	kJ/mol	Joback Method
hvap	44.14	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	5.173		Crippen Method
mcvol	194.030	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	1270.83		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1271.05		NIST Webbook
rinpol	1271.47		NIST Webbook
rinpol	1271.70		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1271.24		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1272.10		NIST Webbook

rinpol	1271.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1271.15		NIST Webbook
tb	496.40	K	Joback Method
tc	659.72	K	Joback Method
tf	212.30 ± 2.00	K	NIST Webbook
tf	213.70 ± 5.00	K	NIST Webbook
vc	0.757	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.81	J/mol×K	659.72	Joback Method
cpg	455.59	J/mol×K	496.40	Joback Method
cpg	473.45	J/mol×K	523.62	Joback Method
cpg	490.62	J/mol×K	550.84	Joback Method
cpg	507.13	J/mol×K	578.06	Joback Method
cpg	522.98	J/mol×K	605.28	Joback Method
cpg	538.20	J/mol×K	632.50	Joback Method
dvisc	0.0001881	Paxs	496.40	Joback Method
dvisc	0.0096568	Paxs	221.27	Joback Method
dvisc	0.0028515	Paxs	267.12	Joback Method
dvisc	0.0012038	Paxs	312.98	Joback Method
dvisc	0.0006335	Paxs	358.83	Joback Method
dvisc	0.0003856	Paxs	404.69	Joback Method
dvisc	0.0002596	Paxs	450.54	Joback Method
hvapt	51.40	kJ/mol	438.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42335e+01
Coeff. B	-3.88952e+03

Coeff. C	-9.89300e+01
Temperature range (K), min.	377.83
Temperature range (K), max.	534.88

Sources

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=C17312571&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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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