

Dodecane, 2,6,11-trimethyl-

Other names:	2,6,11-Trimethyldodecane
Inchi:	InChI=1S/C15H32/c1-13(2)9-6-7-11-15(5)12-8-10-14(3)4/h13-15H,6-12H2,1-5H3
InchiKey:	FONXOARHSFUBAN-UHFFFAOYSA-N
Formula:	C15H32
SMILES:	CC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]:	212.41
CAS:	31295-56-4

Physical Properties

Property code	Value	Unit	Source
gf	68.10	kJ/mol	Joback Method
hf	-368.77	kJ/mol	Joback Method
hfus	24.04	kJ/mol	Joback Method
hvap	47.82	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.665		Crippen Method
mcvol	222.210	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	1275.00		NIST Webbook
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tb	541.28	K	Joback Method
tc	708.78	K	Joback Method
tf	213.81	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.60	J/molxK	541.28	Joback Method
cpg	578.41	J/molxK	569.20	Joback Method
cpg	597.41	J/molxK	597.11	Joback Method
cpg	615.63	J/molxK	625.03	Joback Method
cpg	633.08	J/molxK	652.95	Joback Method
cpg	649.78	J/molxK	680.87	Joback Method

cpg	665.77	J/mol×K	708.78	Joback Method
dvisc	0.0251735	Paxs	213.81	Joback Method
dvisc	0.0043898	Paxs	268.39	Joback Method
dvisc	0.0013813	Paxs	322.97	Joback Method
dvisc	0.0006072	Paxs	377.54	Joback Method
dvisc	0.0003285	Paxs	432.12	Joback Method
dvisc	0.0002040	Paxs	486.70	Joback Method
dvisc	0.0001394	Paxs	541.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31295564&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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