Dodecane, 5-methyl-

Other names: 5-Methyldodecane
Inchi: InChI=1S/C13H28/c1-4-6-8-9-10-12-13(3)11-7-5-2/h13H,4-12H2,1-3H3
InchiKey: NVINYZLICSJRSI-UHFFFAOYSA-N
Formula: C13H28
SMILES: CCCCCCCC(C)CCCC
Mol. weight [g/mol]: 184.36
CAS: 17453-93-9

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	1248.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1255.93		NIST Webbook
rinpol	1255.93		NIST Webbook
rinpol	1255.85		NIST Webbook
rinpol	1255.27		NIST Webbook
rinpol	1255.07		NIST Webbook
rinpol	1255.16		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1256.20		NIST Webbook

rinpol	1253.00		NIST Webbook
tb	496.40	K	Joback Method
tc	659.72	K	Joback Method
tf	203.60 ± 2.00	K	NIST Webbook
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	552.81	J/mol×K	659.72	Joback Method
dvisc	0.0096568	Pa×s	221.27	Joback Method
dvisc	0.0028515	Pa×s	267.12	Joback Method
dvisc	0.0012038	Pa×s	312.98	Joback Method
dvisc	0.0006335	Pa×s	358.83	Joback Method
dvisc	0.0003856	Pa×s	404.69	Joback Method
dvisc	0.0002596	Pa×s	450.54	Joback Method
dvisc	0.0001881	Pa×s	496.40	Joback Method
hvapt	50.60	kJ/mol	434.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.68022e+01
Coeff. B	-6.07445e+03
Coeff. C	-1.12100e+00
Temperature range (K), min.	368.94
Temperature range (K), max.	529.76

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17453939&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume