

2-METHYL-1-DODECENE

Inchi:	InChI=1S/C13H26/c1-4-5-6-7-8-9-10-11-12-13(2)3/h2,4-12H2,1,3H3
InchiKey:	PWRBDKMPAZFCSV-UHFFFAOYSA-N
Formula:	C13H26
SMILES:	C=C(C)CCCCCCCCC
Mol. weight [g/mol]:	182.35
CAS:	16435-49-7

Physical Properties

Property code	Value	Unit	Source
af	0.5733		Cheméo Relay (1.0)
gf	137.87	kJ/mol	Joback Method
hf	-214.62	kJ/mol	Cheméo Relay (1.0)
hfus	26.84	kJ/mol	Joback Method
hvap	61.45	kJ/mol	Cheméo Relay (1.0)
ie	9.15	eV	Cheméo Relay (1.0)
log10ws	-6.35		Cheméo Relay (1.0)
logp	5.093		Crippen Method
mcvol	189.730	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook
tb	496.86	K	Cheméo Relay (1.0)
tc	663.31	K	Cheméo Relay (1.0)
tf	252.24	K	Cheméo Relay (1.0)
vc	0.740	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.75	J/mol×K	493.40	Joback Method
cpg	454.03	J/mol×K	521.02	Joback Method
cpg	470.61	J/mol×K	548.64	Joback Method
cpg	486.52	J/mol×K	576.26	Joback Method
cpg	501.78	J/mol×K	603.88	Joback Method

cpg	516.41	J/mol×K	631.49	Joback Method
cpg	530.43	J/mol×K	659.11	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49958e+01
Coeff. B	-4.36722e+03
Coeff. C	-7.80970e+01
Temperature range (K), min.	375.02
Temperature range (K), max.	529.05

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16435497&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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