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)CCCCCCCCCC
Mol. weight [g/mol]: 182.35
CAS: 16435-49-7

Physical Properties

Property code	Value	Unit	Source
gf	137.87	kJ/mol	Joback Method
hf	-196.01	kJ/mol	Joback Method
hfus	26.84	kJ/mol	Joback Method
hvap	43.94	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	5.093		Crippen Method
mcvol	189.730	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	1285.00		NIST Webbook
tb	493.40	K	Joback Method
tc	659.11	K	Joback Method
tf	220.55	K	Joback Method
vc	0.746	m3/kmol	Joback Method

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(Pvp) = 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

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=C16435497&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

Legend

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
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