2-Methyl-1-tridecene

Other names: 1-Tridecene, 2-methyl-
Inchi: InChI=1S/C14H28/c1-4-5-6-7-8-9-10-11-12-13-14(2)3/h2,4-13H2,1,3H3
InchiKey: VNBHQOHLCULRDN-UHFFFAOYSA-N
Formula: C14H28
SMILES: C=C(C)CCCCCCCCCCC
Mol. weight [g/mol]: 196.38
CAS: 18094-01-4

Physical Properties

Property code	Value	Unit	Source
af	0.6105		Cheméo Relay (1.0)
gf	146.29	kJ/mol	Joback Method
hf	-236.69	kJ/mol	Cheméo Relay (1.0)
hfus	29.43	kJ/mol	Joback Method
hvap	66.13	kJ/mol	Cheméo Relay (1.0)
ie	9.18	eV	Cheméo Relay (1.0)
log10ws	-6.64		Cheméo Relay (1.0)
logp	5.483		Crippen Method
mcvol	203.820	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1386.00		NIST Webbook
tb	514.89	K	Cheméo Relay (1.0)
tc	679.07	K	Cheméo Relay (1.0)
tf	261.84	K	Cheméo Relay (1.0)
vc	0.797	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.39	J/mol×K	516.28	Joback Method
cpg	504.30	J/mol×K	543.74	Joback Method
cpg	521.48	J/mol×K	571.19	Joback Method
cpg	537.97	J/mol×K	598.65	Joback Method

cpg	553.77	J/mol×K	626.11	Joback Method
cpg	568.92	J/mol×K	653.56	Joback Method
cpg	583.44	J/mol×K	681.02	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55791e+01
Coeff. B	-4.76568e+03
Coeff. C	-8.16500e+01
Temperature range (K), min.	393.30
Temperature range (K), max.	545.80

Sources

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=C18094014&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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