3-Undecyne

Other names: 3-C11H20
Inchi: InChI=1S/C11H20/c1-3-5-7-9-11-10-8-6-4-2/h3-5,7,9-11H2,1-2H3
InchiKey: DPWGJNPCPLQVKQ-UHFFFAOYSA-N
Formula: C11H20
SMILES: CCC#CCCCCCCC
Mol. weight [g/mol]: 152.28
CAS: 60212-30-8

Physical Properties

Property code	Value	Unit	Source
gf	244.54	kJ/mol	Joback Method
hf	1.93	kJ/mol	Joback Method
hfus	27.37	kJ/mol	Joback Method
hvap	42.23	kJ/mol	Joback Method
ie	9.17 ± 0.02	eV	NIST Webbook
log10ws	-4.22		Crippen Method
logp	3.760		Crippen Method
mcvol	157.250	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1112.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1112.00		NIST Webbook
ripol	1283.80		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1301.30		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1306.00		NIST Webbook
ripol	1301.30		NIST Webbook
ripol	1285.80		NIST Webbook

ripol	1300.00		NIST Webbook
ripol	1306.00		NIST Webbook
ripol	1306.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1281.10		NIST Webbook
ripol	1306.00		NIST Webbook
ripol	1306.00		NIST Webbook
tb	460.08	K	Joback Method
tc	642.86	K	Joback Method
tf	319.83	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.56	J/mol×K	460.08	Joback Method
cpg	347.02	J/mol×K	490.54	Joback Method
cpg	361.85	J/mol×K	521.01	Joback Method
cpg	376.06	J/mol×K	551.47	Joback Method
cpg	389.69	J/mol×K	581.93	Joback Method
cpg	402.74	J/mol×K	612.39	Joback Method
cpg	415.23	J/mol×K	642.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.00 ± 1.00	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54172e+01
Coeff. B	-4.32455e+03

Coeff. C	-7.26860e+01
Temperature range (K), min.	358.52
Temperature range (K), max.	500.62

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60212308&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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