Undecane, 2,6,10-trimethyl

Other names: Undecane, 2,6,10-trimethyl, isomer # 1
Inchi: InChI=1S/C14H30/c1-12(2)8-6-10-14(5)11-7-9-13(3)4/h12-14H,6-11H2,1-5H3
InchiKey: RMDGVETXJWRSGT-UHFFFAOYSA-N
Formula: C14H30
SMILES: CC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 198.39

Physical Properties

Property code	Value	Unit	Source
gf	59.68	kJ/mol	Joback Method
hf	-348.13	kJ/mol	Joback Method
hfus	21.45	kJ/mol	Joback Method
hvap	45.59	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	5.275		Crippen Method
mcvol	208.120	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
rinpol	1260.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1261.00		NIST Webbook

rinpol	1275.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1260.00		NIST Webbook
tb	518.40	K	Joback Method
tc	686.98	K	Joback Method
tf	202.54	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.37	J/mol×K	518.40	Joback Method
cpg	525.66	J/mol×K	546.50	Joback Method
cpg	544.17	J/mol×K	574.59	Joback Method
cpg	561.92	J/mol×K	602.69	Joback Method
cpg	578.93	J/mol×K	630.79	Joback Method
cpg	595.22	J/mol×K	658.88	Joback Method
cpg	610.81	J/mol×K	686.98	Joback Method
dvisc	0.0290632	Pa×s	202.54	Joback Method
dvisc	0.0049284	Pa×s	255.18	Joback Method
dvisc	0.0015334	Pa×s	307.83	Joback Method
dvisc	0.0006710	Pa×s	360.47	Joback Method
dvisc	0.0003624	Pa×s	413.11	Joback Method
dvisc	0.0002250	Pa×s	465.76	Joback Method
dvisc	0.0001539	Pa×s	518.40	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R12131&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume