

Undecane, 4,6,8-trimethyl, # 3

Inchi:	InChI=1S/C14H30/c1-6-8-12(3)10-14(5)11-13(4)9-7-2/h12-14H,6-11H2,1-5H3
InchiKey:	AGDLQJZTKSGOKD-UHFFFAOYSA-N
Formula:	C14H30
SMILES:	CCCC(C)CC(C)CC(C)CCC
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	1258.00		NIST Webbook
rinpol	1258.00		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	595.22	J/mol×K	658.88	Joback Method
cpg	578.93	J/mol×K	630.79	Joback Method
cpg	561.92	J/mol×K	602.69	Joback Method
cpg	544.17	J/mol×K	574.59	Joback Method
cpg	525.66	J/mol×K	546.50	Joback Method
cpg	610.81	J/mol×K	686.98	Joback Method
dvisc	0.0001539	Pa×s	518.40	Joback Method

dvisc	0.0002250	Pa×s	465.76	Joback Method
dvisc	0.0003624	Pa×s	413.11	Joback Method
dvisc	0.0006710	Pa×s	360.47	Joback Method
dvisc	0.0015334	Pa×s	307.83	Joback Method
dvisc	0.0049284	Pa×s	255.18	Joback Method
dvisc	0.0290632	Pa×s	202.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R568577&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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