

2-Undecene, 4,6,8-trimethyl

Inchi:

LnChI=1S/C14H28/c1-6-8-12(3)10-14(5)11-13(4)9-7-2/h6,8,12-14H,7,9-11H2,1-5H3/b8-6

InchiKey:

XLHHFMMDEMBZND-SOFGYWHQSA-N

Formula:

C14H28

SMILES:

CC=CC(C)CC(C)CC(C)CCC

Mol. weight [g/mol]:

196.37

Physical Properties

Property code	Value	Unit	Source
gf	139.90	kJ/mol	Joback Method
hf	-230.91	kJ/mol	Joback Method
hfus	21.65	kJ/mol	Joback Method
hvap	45.55	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	5.051		Crippen Method
mcvol	203.820	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	1220.00		NIST Webbook
tb	522.56	K	Joback Method
tc	698.17	K	Joback Method
tf	197.46	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.43	J/mol×K	522.56	Joback Method
cpg	576.74	J/mol×K	668.90	Joback Method
cpg	560.86	J/mol×K	639.63	Joback Method
cpg	544.22	J/mol×K	610.36	Joback Method
cpg	526.79	J/mol×K	581.10	Joback Method
cpg	508.54	J/mol×K	551.83	Joback Method
cpg	591.89	J/mol×K	698.17	Joback Method
dvisc	0.0001301	Pa×s	522.56	Joback Method
dvisc	0.0001903	Pa×s	468.38	Joback Method

dvisc	0.0003074	Pa×s	414.19	Joback Method
dvisc	0.0005740	Pa×s	360.01	Joback Method
dvisc	0.0013372	Pa×s	305.83	Joback Method
dvisc	0.0044836	Pa×s	251.64	Joback Method
dvisc	0.0292014	Pa×s	197.46	Joback Method

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=R568364&Units=SI

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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