

Hexane, 3,4-diethyl-2,2,5,5-tetramethyl-, (R*,R*)-(+/-)-

Inchi:	InChI=1S/C14H30/c1-9-11(13(3,4)5)12(10-2)14(6,7)8/h11-12H,9-10H2,1-8H3
InchiKey:	FMTQAAHAQDKAMI-UHFFFAOYSA-N
Formula:	C14H30
SMILES:	CCC(C(CC)C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]:	198.39
CAS:	112655-34-2

Physical Properties

Property code	Value	Unit	Source
gf	67.80	kJ/mol	Joback Method
hf	-360.35	kJ/mol	Joback Method
hfus	10.14	kJ/mol	Joback Method
hvap	43.39	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	5.131		Crippen Method
mcvol	208.120	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
tb	512.38	K	Joback Method
tc	696.94	K	Joback Method
tf	222.38	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.84	J/molxK	512.38	Joback Method
cpg	532.32	J/molxK	543.14	Joback Method
cpg	552.66	J/molxK	573.90	Joback Method
cpg	571.92	J/molxK	604.66	Joback Method
cpg	590.14	J/molxK	635.42	Joback Method
cpg	607.38	J/molxK	666.18	Joback Method
cpg	623.69	J/molxK	696.94	Joback Method
dvisc	0.0389132	Paxs	222.38	Joback Method
dvisc	0.0067312	Paxs	270.71	Joback Method

dvisc	0.0019814	Paxs	319.05	Joback Method
dvisc	0.0008046	Paxs	367.38	Joback Method
dvisc	0.0004029	Paxs	415.71	Joback Method
dvisc	0.0002330	Paxs	464.05	Joback Method
dvisc	0.0001494	Paxs	512.38	Joback Method

Sources

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=C112655342&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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