

Octane, 4,5-dipropyl-

Inchi:	InChI=1S/C14H30/c1-5-9-13(10-6-2)14(11-7-3)12-8-4/h13-14H,5-12H2,1-4H3
InchiKey:	QGEPIAWTQXRCGQ-UHFFFAOYSA-N
Formula:	C14H30
SMILES:	CCCC(CCC)C(CCC)CCC
Mol. weight [g/mol]:	198.39
CAS:	20905-05-9

Physical Properties

Property code	Value	Unit	Source
gf	62.12	kJ/mol	Joback Method
hf	-342.85	kJ/mol	Joback Method
hfus	24.97	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	5.419		Crippen Method
mcvol	208.120	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
rinpol	1226.00		NIST Webbook
rinpol	1226.00		NIST Webbook
tb	493.00 ± 2.00	K	NIST Webbook
tc	684.31	K	Joback Method
tf	217.54	K	Joback Method
vc	0.807	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.22	J/mol×K	518.84	Joback Method
cpg	525.09	J/mol×K	546.42	Joback Method
cpg	543.22	J/mol×K	574.00	Joback Method
cpg	560.62	J/mol×K	601.58	Joback Method
cpg	577.31	J/mol×K	629.15	Joback Method
cpg	593.31	J/mol×K	656.73	Joback Method
cpg	608.64	J/mol×K	684.31	Joback Method

dvisc	0.0154332	Paxs	217.54	Joback Method
dvisc	0.0035509	Paxs	267.76	Joback Method
dvisc	0.0012995	Paxs	317.97	Joback Method
dvisc	0.0006256	Paxs	368.19	Joback Method
dvisc	0.0003589	Paxs	418.41	Joback Method
dvisc	0.0002320	Paxs	468.62	Joback Method
dvisc	0.0001631	Paxs	518.84	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=C20905059&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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