

Dodecane, 6-ethyl

Inchi:	InChI=1S/C14H30/c1-4-7-9-11-13-14(6-3)12-10-8-5-2/h14H,4-13H2,1-3H3
InchiKey:	NHGKHDNTGOKJAX-UHFFFAOYSA-N
Formula:	C14H30
SMILES:	CCCCCCC(CC)CCCC
Mol. weight [g/mol]:	198.39

Physical Properties

Property code	Value	Unit	Source
gf	64.56	kJ/mol	Joback Method
hf	-337.57	kJ/mol	Joback Method
hfus	28.49	kJ/mol	Joback Method
hvap	46.37	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	5.563		Crippen Method
mcvol	208.120	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	1326.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1336.00		NIST Webbook
tb	519.28	K	Joback Method
tc	681.76	K	Joback Method
tf	232.54	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.07	J/molxK	519.28	Joback Method
cpg	591.46	J/molxK	654.68	Joback Method
cpg	575.74	J/molxK	627.60	Joback Method
cpg	559.36	J/molxK	600.52	Joback Method
cpg	542.30	J/molxK	573.44	Joback Method
cpg	524.54	J/molxK	546.36	Joback Method

cpg	606.55	J/molxK	681.76	Joback Method
dvisc	0.0001730	Paxs	519.28	Joback Method
dvisc	0.0002394	Paxs	471.49	Joback Method
dvisc	0.0003567	Paxs	423.70	Joback Method
dvisc	0.0005882	Paxs	375.91	Joback Method
dvisc	0.0011218	Paxs	328.12	Joback Method
dvisc	0.0026666	Paxs	280.33	Joback Method
dvisc	0.0090478	Paxs	232.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R8732&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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