

Dodecane, 6-methyl-5-propyl

Inchi:	InChI=1S/C16H34/c1-5-8-10-11-13-15(4)16(12-7-3)14-9-6-2/h15-16H,5-14H2,1-4H3
InchiKey:	YUQIWBNAPEJSR-UHFFFAOYSA-N
Formula:	C16H34
SMILES:	CCCCCCC(C)C(CCC)CCCC
Mol. weight [g/mol]:	226.44

Physical Properties

Property code	Value	Unit	Source
gf	78.96	kJ/mol	Joback Method
hf	-384.13	kJ/mol	Joback Method
hfus	30.15	kJ/mol	Joback Method
hvap	50.43	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	6.199		Crippen Method
mcvol	236.300	ml/mol	McGowan Method
pc	1333.93	kPa	Joback Method
rinpol	1453.00		NIST Webbook
tb	564.60	K	Joback Method
tc	728.45	K	Joback Method
tf	240.08	K	Joback Method
vc	0.919	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.18	J/molxK	564.60	Joback Method
cpg	703.80	J/molxK	701.14	Joback Method
cpg	686.99	J/molxK	673.83	Joback Method
cpg	669.44	J/molxK	646.53	Joback Method
cpg	651.14	J/molxK	619.22	Joback Method
cpg	632.06	J/molxK	591.91	Joback Method
cpg	719.89	J/molxK	728.45	Joback Method
dvisc	0.0001338	Paxs	564.60	Joback Method
dvisc	0.0001908	Paxs	510.51	Joback Method

dvisc	0.0002961	Paxs	456.43	Joback Method
dvisc	0.0005170	Paxs	402.34	Joback Method
dvisc	0.0010735	Paxs	348.25	Joback Method
dvisc	0.0029159	Paxs	294.17	Joback Method
dvisc	0.0124242	Paxs	240.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R9042&Units=SI
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

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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