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: YUQIWBNAPXEJSR-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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.18	J/mol×K	564.60	Joback Method
cpg	632.06	J/mol×K	591.91	Joback Method
cpg	651.14	J/mol×K	619.22	Joback Method
cpg	669.44	J/mol×K	646.53	Joback Method
cpg	686.99	J/mol×K	673.83	Joback Method
cpg	703.80	J/mol×K	701.14	Joback Method
cpg	719.89	J/mol×K	728.45	Joback Method
dvisc	0.0124242	Pa×s	240.08	Joback Method
dvisc	0.0029159	Pa×s	294.17	Joback Method

dvisc	0.0010735	Pa×s	348.25	Joback Method
dvisc	0.0005170	Pa×s	402.34	Joback Method
dvisc	0.0002961	Pa×s	456.43	Joback Method
dvisc	0.0001908	Pa×s	510.51	Joback Method
dvisc	0.0001338	Pa×s	564.60	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=R9042&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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