

Dodecane, 5-butyl

Inchi:	InChI=1S/C16H34/c1-4-7-10-11-12-15-16(13-8-5-2)14-9-6-3/h16H,4-15H2,1-3H3
InchiKey:	QYYBGSJTXXHPEE-UHFFFAOYSA-N
Formula:	C16H34
SMILES:	CCCCCCCC(CCCC)CCCC
Mol. weight [g/mol]:	226.44

Physical Properties

Property code	Value	Unit	Source
gf	81.40	kJ/mol	Joback Method
hf	-378.85	kJ/mol	Joback Method
hfus	33.67	kJ/mol	Joback Method
hvap	50.82	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	6.344		Crippen Method
mvol	236.300	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
tb	565.04	K	Joback Method
tc	726.28	K	Joback Method
tf	255.08	K	Joback Method
vc	0.925	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.96	J/molxK	565.04	Joback Method
cpg	631.47	J/molxK	591.91	Joback Method
cpg	650.21	J/molxK	618.79	Joback Method
cpg	668.20	J/molxK	645.66	Joback Method
cpg	685.47	J/molxK	672.53	Joback Method
cpg	702.03	J/molxK	699.40	Joback Method
cpg	717.90	J/molxK	726.28	Joback Method
dvisc	0.0077044	Paxs	255.08	Joback Method
dvisc	0.0022640	Paxs	306.74	Joback Method
dvisc	0.0009470	Paxs	358.40	Joback Method

dvisc	0.0004934	Paxs	410.06	Joback Method
dvisc	0.0002974	Paxs	461.72	Joback Method
dvisc	0.0001985	Paxs	513.38	Joback Method
dvisc	0.0001427	Paxs	565.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R8703&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

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
hvac:	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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