

3,3-Diethylundecane

Inchi:	InChI=1S/C15H32/c1-5-9-10-11-12-13-14-15(6-2,7-3)8-4/h5-14H2,1-4H3
InchiKey:	JRKHGXZNVIUSTG-UHFFFAOYSA-N
Formula:	C15H32
SMILES:	CCCCCCCCC(CC)(CC)CC
Mol. weight [g/mol]:	212.41

Physical Properties

Property code	Value	Unit	Source
gf	78.26	kJ/mol	Joback Method
hf	-361.68	kJ/mol	Joback Method
hfus	27.19	kJ/mol	Joback Method
hvap	47.69	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.953		Crippen Method
mcvol	222.210	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	1449.00		NIST Webbook
tb	539.37	K	Joback Method
tc	706.24	K	Joback Method
tf	261.23	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.41	J/mol×K	539.37	Joback Method
cpg	650.51	J/mol×K	678.43	Joback Method
cpg	634.09	J/mol×K	650.62	Joback Method
cpg	616.91	J/mol×K	622.80	Joback Method
cpg	598.92	J/mol×K	594.99	Joback Method
cpg	580.10	J/mol×K	567.18	Joback Method
cpg	666.20	J/mol×K	706.24	Joback Method
dvisc	0.0001565	Pa×s	539.37	Joback Method
dvisc	0.0002204	Pa×s	493.01	Joback Method

dvisc	0.0003332	Pa×s	446.66	Joback Method
dvisc	0.0005544	Pa×s	400.30	Joback Method
dvisc	0.0010539	Pa×s	353.94	Joback Method
dvisc	0.0024315	Pa×s	307.59	Joback Method
dvisc	0.0075476	Pa×s	261.23	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=R415235&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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