

Pregeijerene

Inchi:	InChI=1S/C12H18/c1-11-7-4-3-5-8-12(2)10-6-9-11/h3-4,7,10H,5-6,8-9H2,1-2H3/b4-3-,11
InchiKey:	ACTKFDMFHYIKRY-KCWZREBISA-N
Formula:	C12H18
SMILES:	CC1=CC=CCCC(C)=CCC1
Mol. weight [g/mol]:	162.27

Physical Properties

Property code	Value	Unit	Source
gf	104.54	kJ/mol	Joback Method
hf	-90.59	kJ/mol	Joback Method
hfus	12.09	kJ/mol	Joback Method
hvap	45.93	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.009		Crippen Method
mvol	156.180	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1288.00		NIST Webbook
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tb	522.70	K	Joback Method
tc	755.05	K	Joback Method
tf	249.86	K	Joback Method
vc	0.568	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.81	J/mol×K	522.70	Joback Method
cpg	440.11	J/mol×K	716.33	Joback Method
cpg	423.95	J/mol×K	677.60	Joback Method
cpg	406.64	J/mol×K	638.88	Joback Method
cpg	388.19	J/mol×K	600.15	Joback Method
cpg	368.58	J/mol×K	561.43	Joback Method
cpg	455.13	J/mol×K	755.05	Joback Method
dvisc	0.0000850	Paxs	522.70	Joback Method

dvisc	0.0001288	Paxs	477.23	Joback Method
dvisc	0.0002128	Paxs	431.75	Joback Method
dvisc	0.0003958	Paxs	386.28	Joback Method
dvisc	0.0008688	Paxs	340.81	Joback Method
dvisc	0.0024293	Paxs	295.33	Joback Method
dvisc	0.0098765	Paxs	249.86	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=R626594&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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