Cyclohexene, 3-pentyl-

Other names: 3-Pentyl-1-cyclohexene
Inchi: InChI=1S/C11H20/c1-2-3-5-8-11-9-6-4-7-10-11/h6,9,11H,2-5,7-8,10H2,1H3
InchiKey: OUBDONKLEWYBJJ-UHFFFAOYSA-N
Formula: C11H20
SMILES: CCCCCC1C=CCCC1
Mol. weight [g/mol]: 152.28

Physical Properties

Property code	Value	Unit	Source
af	0.3506		Cheméo Relay (1.0)
gf	96.15	kJ/mol	Joback Method
hf	-125.53	kJ/mol	Cheméo Relay (1.0)
hfus	17.30	kJ/mol	Joback Method
hvap	52.83	kJ/mol	Cheméo Relay (1.0)
ie	8.82	eV	Cheméo Relay (1.0)
log10ws	-5.33		Cheméo Relay (1.0)
logp	3.923		Crippen Method
mcvol	150.690	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	1144.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1298.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1306.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1276.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1287.00		NIST Webbook
ripol	1292.00		NIST Webbook
ripol	1270.40		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1275.90		NIST Webbook
ripol	1281.60		NIST Webbook
ripol	1287.00		NIST Webbook

ripol	1292.30		NIST Webbook
ripol	1298.00		NIST Webbook
ripol	1264.60		NIST Webbook
tb	471.41	K	Cheméo Relay (1.0)
tc	656.88	K	Cheméo Relay (1.0)
tf	207.72	K	Cheméo Relay (1.0)
vc	0.556	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-6.49360e+01
Coeff. B	1.11492e+00
Coeff. C	-6.42880e-04
Coeff. D	1.33500e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.12383e+01
Coeff. B	1.37471e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	221.87
Temperature range (K), max.	466.58

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15232925&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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