

5-Pentylcyclohexa-1,3-diene

Inchi:	InChI=1S/C11H18/c1-2-3-5-8-11-9-6-4-7-10-11/h4,6-7,9,11H,2-3,5,8,10H2,1H3
InchiKey:	PPCHPNONKYLBQT-UHFFFAOYSA-N
Formula:	C11H18
SMILES:	CCCCC1C=CC=CC1
Mol. weight [g/mol]:	150.26
CAS:	56318-84-4

Physical Properties

Property code	Value	Unit	Source
gf	126.11	kJ/mol	Joback Method
hf	-100.49	kJ/mol	Joback Method
hfus	18.52	kJ/mol	Joback Method
hvap	41.09	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.699		Crippen Method
mcvol	146.390	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
rinpol	1161.10		NIST Webbook
rinpol	1161.10		NIST Webbook
tb	468.95	K	Joback Method
tc	667.36	K	Joback Method
tf	222.63	K	Joback Method
vc	0.556	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.04	J/mol×K	468.95	Joback Method
cpg	333.05	J/mol×K	502.02	Joback Method
cpg	350.13	J/mol×K	535.09	Joback Method
cpg	366.31	J/mol×K	568.15	Joback Method
cpg	381.63	J/mol×K	601.22	Joback Method
cpg	396.12	J/mol×K	634.29	Joback Method
cpg	409.80	J/mol×K	667.36	Joback Method

dvisc	0.0049179	Paxs	222.63	Joback Method
dvisc	0.0020107	Paxs	263.68	Joback Method
dvisc	0.0010461	Paxs	304.74	Joback Method
dvisc	0.0006356	Paxs	345.79	Joback Method
dvisc	0.0004292	Paxs	386.84	Joback Method
dvisc	0.0003126	Paxs	427.90	Joback Method
dvisc	0.0002406	Paxs	468.95	Joback Method

Sources

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=C56318844&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	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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