

Cyclopentylcycloheptane

Inchi:	InChI=1S/C12H22/c1-2-4-8-11(7-3-1)12-9-5-6-10-12/h11-12H,1-10H2
InchiKey:	IVZDBCJTKAVJQI-UHFFFAOYSA-N
Formula:	C12H22
SMILES:	C1CCCC(C2CCCC2)CC1
Mol. weight [g/mol]:	166.30
CAS:	42347-48-8

Physical Properties

Property code	Value	Unit	Source
chl	-7640.00 ± 4.00	kJ/mol	NIST Webbook
gf	99.06	kJ/mol	Joback Method
hf	-182.37	kJ/mol	Joback Method
hfus	10.51	kJ/mol	Joback Method
hvap	43.16	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	4.147		Crippen Method
mcvol	158.220	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1342.00		NIST Webbook
rinpol	1310.00		NIST Webbook
tb	513.06	K	Joback Method
tc	745.11	K	Joback Method
tf	239.76	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.05	J/molxK	513.06	Joback Method
cpg	411.12	J/molxK	551.73	Joback Method
cpg	435.56	J/molxK	590.41	Joback Method
cpg	458.45	J/molxK	629.08	Joback Method
cpg	479.81	J/molxK	667.76	Joback Method
cpg	499.72	J/molxK	706.43	Joback Method

cpg	518.21	J/mol×K	745.11	Joback Method
dvisc	0.0108669	Paxs	239.76	Joback Method
dvisc	0.0035294	Paxs	285.31	Joback Method
dvisc	0.0015623	Paxs	330.86	Joback Method
dvisc	0.0008424	Paxs	376.41	Joback Method
dvisc	0.0005190	Paxs	421.96	Joback Method
dvisc	0.0003514	Paxs	467.51	Joback Method
dvisc	0.0002550	Paxs	513.06	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42347488&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
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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