

Cyclododecane, 1,1,4,4-tetramethyl-

Inchi:	InChI=1S/C16H32/c1-15(2)11-9-7-5-6-8-10-12-16(3,4)14-13-15/h5-14H2,1-4H3
InchiKey:	DGZRYHBSBBFPHU-UHFFFAOYSA-N
Formula:	C16H32
SMILES:	CC1(C)CCCCCCCCC(C)(C)CC1
Mol. weight [g/mol]:	224.43
CAS:	20250-91-3

Physical Properties

Property code	Value	Unit	Source
gf	17.00	kJ/mol	Joback Method
hf	-346.07	kJ/mol	Joback Method
hfus	4.91	kJ/mol	Joback Method
hvap	50.06	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.953		Crippen Method
mcvol	225.440	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
tb	606.46	K	Joback Method
tc	847.16	K	Joback Method
tf	299.90	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.82	J/molxK	606.46	Joback Method
cpg	647.78	J/molxK	646.58	Joback Method
cpg	676.00	J/molxK	686.69	Joback Method
cpg	702.71	J/molxK	726.81	Joback Method
cpg	728.13	J/molxK	766.93	Joback Method
cpg	752.49	J/molxK	807.04	Joback Method
cpg	776.01	J/molxK	847.16	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=C20250913&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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