

Cyclododecylbenzene

Inchi:	InChI=1S/C18H28/c1-2-4-6-9-13-17(14-10-7-5-3-1)18-15-11-8-12-16-18/h8,11-12,15-17H
InchiKey:	NKFNKCCQNUBQGQP-UHFFFAOYSA-N
Formula:	C18H28
SMILES:	c1ccc(C2CCCCCCCCCCCC2)cc1
Mol. weight [g/mol]:	244.41
CAS:	15971-88-7

Physical Properties

Property code	Value	Unit	Source
gf	164.94	kJ/mol	Joback Method
hf	-160.96	kJ/mol	Joback Method
hfus	15.65	kJ/mol	Joback Method
hvap	59.40	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	6.075		Crippen Method
mcvol	229.860	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
tb	683.09	K	Joback Method
tc	943.78	K	Joback Method
tf	305.30	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.59	J/mol×K	683.09	Joback Method
cpg	696.90	J/mol×K	726.54	Joback Method
cpg	723.70	J/mol×K	769.99	Joback Method
cpg	748.04	J/mol×K	813.43	Joback Method
cpg	769.94	J/mol×K	856.88	Joback Method
cpg	789.43	J/mol×K	900.33	Joback Method
cpg	806.54	J/mol×K	943.78	Joback Method
dvisc	0.0105681	Pa×s	305.30	Joback Method
dvisc	0.0015365	Pa×s	368.26	Joback Method

dvisc	0.0003923	Pa×s	431.23	Joback Method
dvisc	0.0001418	Pa×s	494.19	Joback Method
dvisc	0.0000645	Pa×s	557.16	Joback Method
dvisc	0.0000345	Pa×s	620.12	Joback Method
dvisc	0.0000207	Pa×s	683.09	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=C15971887&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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