

1,2,6,7-Cyclodecatetraene

Inchi: InChI=1S/C10H12/c1-2-4-6-8-10-9-7-5-3-1/h1,5-6,10H,2,4,7,9H2
InchiKey: ADAQQPDXZURMQF-UHFFFAOYSA-N
Formula: C10H12
SMILES: C1=CCCC=C=CCCC=1
Mol. weight [g/mol]: 132.20
CAS: 3451-55-6

Physical Properties

Property code	Value	Unit	Source
chs	-5932.90 ± 3.50	kJ/mol	NIST Webbook
hf	356.10 ± 3.80	kJ/mol	NIST Webbook
hfs	282.80 ± 3.80	kJ/mol	NIST Webbook
hsub	73.30	kJ/mol	NIST Webbook
hsub	73.00 ± 0.40	kJ/mol	NIST Webbook
hsub	73.30 ± 0.40	kJ/mol	NIST Webbook
ie	8.55	eV	NIST Webbook
log10ws	-3.36		Crippen Method
logp	2.983		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
tf	309.00 ± 1.00	K	NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3451556&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion

hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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