

1,2:3,4-Dicyclooctenobenzene

Inchi:	InChI=1S/C18H26/c1-3-7-11-17-15(9-5-1)13-14-16-10-6-2-4-8-12-18(16)17/h13-14H,1-11H
InchiKey:	IRATWOHAZBNERN-UHFFFAOYSA-N
Formula:	C18H26
SMILES:	<chem>c1cc2c(c3c1CCCCC3)CCCCC2</chem>
Mol. weight [g/mol]:	242.40
CAS:	17044-68-7

Physical Properties

Property code	Value	Unit	Source
gf	248.52	kJ/mol	Joback Method
hf	-63.41	kJ/mol	Joback Method
hfus	16.78	kJ/mol	Joback Method
hvap	61.40	kJ/mol	Joback Method
ie	7.93 ± 0.03	eV	NIST Webbook
log10ws	-6.15		Crippen Method
logp	5.005		Crippen Method
mcvol	219.000	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
tb	701.30	K	Joback Method
tc	956.31	K	Joback Method
tf	379.84	K	Joback Method
vc	0.803	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.87	J/mol×K	701.30	Joback Method
cpg	746.22	J/mol×K	913.80	Joback Method
cpg	728.67	J/mol×K	871.30	Joback Method
cpg	709.47	J/mol×K	828.80	Joback Method
cpg	688.51	J/mol×K	786.30	Joback Method
cpg	665.67	J/mol×K	743.80	Joback Method
cpg	762.21	J/mol×K	956.31	Joback Method
dvisc	0.0000919	Paxs	701.30	Joback Method

dvisc	0.0001253	Paxs	647.72	Joback Method
dvisc	0.0001807	Paxs	594.15	Joback Method
dvisc	0.0002801	Paxs	540.57	Joback Method
dvisc	0.0004783	Paxs	486.99	Joback Method
dvisc	0.0009323	Paxs	433.42	Joback Method
dvisc	0.0021933	Paxs	379.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17044687&Units=SI
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

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
ie:	Ionization energy
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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