

Bi-2,4,6-cycloheptatrien-1-yl

Other names:	Bitropenyl Heptafulvalene, dihydro- 7,7'-Bis(cycloheptatrienyl) 7,7'-Ditropyl 7,7'-Bicycloheptatrienyl
Inchi:	InChI=1S/C14H14/c1-2-6-10-13(9-5-1)14-11-7-3-4-8-12-14/h1-14H
InchiKey:	DMVKBMNNLFFZBY-UHFFFAOYSA-N
Formula:	C14H14
SMILES:	<chem>C1=CC=CC(C2C=CC=CC=C2)C=C1</chem>
Mol. weight [g/mol]:	182.26
CAS:	831-18-5

Physical Properties

Property code	Value	Unit	Source
gf	271.46	kJ/mol	Joback Method
hf	110.71	kJ/mol	Joback Method
hfus	18.82	kJ/mol	Joback Method
hvap	49.71	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.583		Crippen Method
mcvol	160.600	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
tb	562.32	K	Joback Method
tc	818.01	K	Joback Method
tf	334.00 ± 1.50	K	NIST Webbook
vc	0.586	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.84	J/mol×K	562.32	Joback Method
cpg	469.50	J/mol×K	775.40	Joback Method
cpg	454.17	J/mol×K	732.78	Joback Method
cpg	437.31	J/mol×K	690.17	Joback Method

cpg	418.84	J/molxK	647.55	Joback Method
cpg	398.71	J/molxK	604.94	Joback Method
cpg	483.36	J/molxK	818.01	Joback Method
dvisc	0.0001444	Paxs	562.32	Joback Method
dvisc	0.0001955	Paxs	511.90	Joback Method
dvisc	0.0002827	Paxs	461.49	Joback Method
dvisc	0.0004477	Paxs	411.07	Joback Method
dvisc	0.0008061	Paxs	360.65	Joback Method
dvisc	0.0017571	Paxs	310.24	Joback Method
dvisc	0.0051829	Paxs	259.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C831185&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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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