1,2:3,4-Dicycloheptenobenzene

Inchi: InChI=1S/C16H22/c1-3-7-13-11-15-9-5-2-6-10-16(15)12-14(13)8-4-1/h11-12H,1-10H2
InchiKey: WJQQTTIQCZWNPU-UHFFFAOYSA-N
Formula: C16H22
SMILES: c1c2c(cc3c1CCCCC3)CCCCC2
Mol. weight [g/mol]: 214.35
CAS: 14314-87-5

Physical Properties

Property code	Value	Unit	Source
gf	255.88	kJ/mol	Joback Method
hf	-9.81	kJ/mol	Joback Method
hfus	15.80	kJ/mol	Joback Method
hvap	56.60	kJ/mol	Joback Method
ie	8.39 ± 0.02	eV	NIST Webbook
log10ws	-5.31		Crippen Method
logp	4.224		Crippen Method
mcvol	190.820	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
tb	647.00	K	Joback Method
tc	896.88	K	Joback Method
tf	364.34	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.13	J/mol×K	647.00	Joback Method
cpg	546.87	J/mol×K	688.65	Joback Method
cpg	567.89	J/mol×K	730.29	Joback Method
cpg	587.31	J/mol×K	771.94	Joback Method
cpg	605.25	J/mol×K	813.59	Joback Method
cpg	621.82	J/mol×K	855.24	Joback Method
cpg	637.14	J/mol×K	896.88	Joback Method
dvisc	0.0023743	Pa×s	364.34	Joback Method

dvisc	0.0012609	Pa×s	411.45	Joback Method
dvisc	0.0007626	Pa×s	458.56	Joback Method
dvisc	0.0005065	Pa×s	505.67	Joback Method
dvisc	0.0003608	Pa×s	552.78	Joback Method
dvisc	0.0002710	Pa×s	599.89	Joback Method
dvisc	0.0002122	Pa×s	647.00	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=C14314875&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
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