Azuleno[2,1,8-ija]azulene,10b,10c-dihydro-

Inchi: InChI=1S/C16H12/c1-2-6-12-10-14-8-4-3-7-13-9-11(5-1)15(12)16(13)14/h1-10,15-16H
InchiKey: BOEDVIFOOMGTJW-UHFFFAOYSA-N
Formula: C16H12
SMILES: C1=CC=C2C=C3C=CC=CC4=CC(=C1)C2C43
Mol. weight [g/mol]: 204.27
CAS: 38765-94-5

Physical Properties

Property code	Value	Unit	Source
gf	465.06	kJ/mol	Joback Method
hf	466.10	kJ/mol	NIST Webbook
hfus	26.19	kJ/mol	Joback Method
hvap	56.86	kJ/mol	Joback Method
ie	7.33 ± 0.03	eV	NIST Webbook
log10ws	-4.59		Crippen Method
logp	3.647		Crippen Method
mcvol	162.760	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
tb	632.90	K	Joback Method
tc	885.04	K	Joback Method
tf	391.64	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.03	J/mol×K	632.90	Joback Method
cpg	433.27	J/mol×K	674.92	Joback Method
cpg	448.10	J/mol×K	716.95	Joback Method
cpg	461.71	J/mol×K	758.97	Joback Method
cpg	474.32	J/mol×K	800.99	Joback Method
cpg	486.11	J/mol×K	843.02	Joback Method
cpg	497.28	J/mol×K	885.04	Joback Method
dvisc	0.0020859	Pa×s	391.64	Joback Method

dvisc	0.0019762	Pa×s	431.85	Joback Method
dvisc	0.0018896	Pa×s	472.06	Joback Method
dvisc	0.0018196	Pa×s	512.27	Joback Method
dvisc	0.0017618	Pa×s	552.48	Joback Method
dvisc	0.0017133	Pa×s	592.69	Joback Method
dvisc	0.0016721	Pa×s	632.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38765945&Units=SI

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