

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

Inchi:	InChI=1S/C17H12/c1-2-6-13-10-15-8-4-3-7-14-9-12(5-1)16(13)11-17(14,15)16/h1-10H,1
InchiKey:	OZYDLMWHHWHGMK-UHFFFAOYSA-N
Formula:	C17H12
SMILES:	C1=CC=C2C=C3C=CC=CC4=CC(=C1)C21CC431
Mol. weight [g/mol]:	216.28
CAS:	38801-41-1

Physical Properties

Property code	Value	Unit	Source
gf	555.16	kJ/mol	Joback Method
hf	407.55	kJ/mol	Joback Method
hfus	17.45	kJ/mol	Joback Method
hvap	56.66	kJ/mol	Joback Method
ie	7.15 ± 0.03	eV	NIST Webbook
log10ws	-4.90		Crippen Method
logp	3.791		Crippen Method
mcvol	165.990	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
tb	659.13	K	Joback Method
tc	926.73	K	Joback Method
tf	479.93	K	Joback Method
vc	0.657	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.76	J/mol×K	659.13	Joback Method
cpg	453.01	J/mol×K	703.73	Joback Method
cpg	466.59	J/mol×K	748.33	Joback Method
cpg	480.15	J/mol×K	792.93	Joback Method
cpg	494.36	J/mol×K	837.53	Joback Method
cpg	509.86	J/mol×K	882.13	Joback Method
cpg	527.34	J/mol×K	926.73	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=C38801411&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
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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