2a,4a,6a,6b-Tetrahydrocyclopenta[cd]pentalene

Other names: Triquinacene
Cyclopenta[cd]pentalene, 2a,4a,6a,6b-tetrahydro-
Inchi: InChI=1S/C10H10/c1-2-8-5-6-9-4-3-7(1)10(8)9/h1-10H
InchiKey: HKRMLKXSBBQRIM-UHFFFAOYSA-N
Formula: C10H10
SMILES: C1=CC2C=CC3C=CC1C23
Mol. weight [g/mol]: 130.19
CAS: 6053-74-3

Physical Properties

Property code	Value	Unit	Source
gf	285.64	kJ/mol	Joback Method
hf	224.00 ± 4.20	kJ/mol	NIST Webbook
hfus	18.70	kJ/mol	Joback Method
hvap	38.33	kJ/mol	Joback Method
ie	8.60	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	-2.29		Crippen Method
logp	2.161		Crippen Method
mcvol	106.280	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
tb	445.50	K	Joback Method
tc	665.95	K	Joback Method
tf	250.80	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.17	J/mol×K	445.50	Joback Method
cpg	245.42	J/mol×K	482.24	Joback Method
cpg	261.26	J/mol×K	518.98	Joback Method
cpg	275.81	J/mol×K	555.73	Joback Method
cpg	289.17	J/mol×K	592.47	Joback Method

cpg	301.45	J/mol×K	629.21	Joback Method
cpg	312.75	J/mol×K	665.95	Joback Method
dvisc	0.0003350	Pa×s	250.80	Joback Method
dvisc	0.0004440	Pa×s	283.25	Joback Method
dvisc	0.0005555	Pa×s	315.70	Joback Method
dvisc	0.0006665	Pa×s	348.15	Joback Method
dvisc	0.0007752	Pa×s	380.60	Joback Method
dvisc	0.0008805	Pa×s	413.05	Joback Method
dvisc	0.0009818	Pa×s	445.50	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6053743&Units=SI
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

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