3(10),4-Caradiene

Inchi: InChI=1S/C10H14/c1-7-4-5-8-9(6-7)10(8,2)3/h4-5,8-9H,1,6H2,2-3H3/t8-,9+/m1/s1
InchiKey: DZRRJUYNXUPJFU-BDAKNGLRSA-N
Formula: C10H14
SMILES: C=C1C=CC2C(C1)C2(C)C
Mol. weight [g/mol]: 134.22

Physical Properties

Property code	Value	Unit	Source
gf	212.56	kJ/mol	Joback Method
hf	26.63	kJ/mol	Joback Method
hfus	10.66	kJ/mol	Joback Method
hvap	36.84	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.775		Crippen Method
mcvol	121.440	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	991.00		NIST Webbook
rinpol	991.00		NIST Webbook
tb	439.84	K	Joback Method
tc	649.54	K	Joback Method
tf	268.92	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.21	J/mol×K	439.84	Joback Method
cpg	275.30	J/mol×K	474.79	Joback Method
cpg	291.05	J/mol×K	509.74	Joback Method
cpg	305.61	J/mol×K	544.69	Joback Method
cpg	319.11	J/mol×K	579.64	Joback Method
cpg	331.68	J/mol×K	614.59	Joback Method
cpg	343.46	J/mol×K	649.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R127572&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume