

C6H5(CHC2H5) radical

Inchi:

lnchl=1S/C9H11/c1-2-6-9-7-4-3-5-8-9/h3-8H,2H2,1H3

InchiKey:

AKVBZJSJOOBLEB-UHFFFAOYSA-N

Formula:

C9H11

SMILES:

CC[CH]c1ccccc1

Mol. weight [g/mol]:

119.18

CAS:

19019-92-2

Physical Properties

Property code	Value	Unit	Source
affp	842.20	kJ/mol	NIST Webbook
basg	809.70	kJ/mol	NIST Webbook
gf	187.25	kJ/mol	Joback Method
hf	57.97	kJ/mol	Joback Method
hfus	11.27	kJ/mol	Joback Method
hvap	37.37	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.649		Crippen Method
mcvol	111.760	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
tb	430.86	K	Joback Method
tc	639.19	K	Joback Method
tf	218.98	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.71	J/mol×K	430.86	Joback Method
cpg	268.18	J/mol×K	604.47	Joback Method
cpg	257.92	J/mol×K	569.75	Joback Method
cpg	246.90	J/mol×K	535.02	Joback Method
cpg	235.07	J/mol×K	500.30	Joback Method
cpg	222.35	J/mol×K	465.58	Joback Method
cpg	277.73	J/mol×K	639.19	Joback Method

dvisc	0.0003521	Pa×s	430.86	Joback Method
dvisc	0.0004134	Pa×s	395.55	Joback Method
dvisc	0.0005010	Pa×s	360.23	Joback Method
dvisc	0.0006329	Pa×s	324.92	Joback Method
dvisc	0.0008466	Pa×s	289.61	Joback Method
dvisc	0.0012276	Pa×s	254.29	Joback Method
dvisc	0.0020068	Pa×s	218.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19019922&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

affp:	Proton affinity
basg:	Gas basicity
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
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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