Benzyl radical

Inchi: InChI=1S/C7H7/c1-7-5-3-2-4-6-7/h2-6H,1H2
InchiKey: SLRMQYXOBQWXCR-UHFFFAOYSA-N
Formula: C7H7
SMILES: [CH2]c1ccccc1
Mol. weight [g/mol]: 91.13
CAS: 2154-56-5

Physical Properties

Property code	Value	Unit	Source
affp	831.40	kJ/mol	NIST Webbook
basg	800.70	kJ/mol	NIST Webbook
ea	1.08	eV	NIST Webbook
ea	2.35 ± 0.07	eV	NIST Webbook
ea	0.89 ± 0.07	eV	NIST Webbook
ea	0.86 ± 0.01	eV	NIST Webbook
ea	0.98 ± 0.09	eV	NIST Webbook
ea	0.76	eV	NIST Webbook
ea	0.91 ± 0.01	eV	NIST Webbook
ea	0.80	eV	NIST Webbook
gf	172.85	kJ/mol	Joback Method
hf	207.00 ± 4.00	kJ/mol	NIST Webbook
hfpi	900.00 ± 6.70	kJ/mol	NIST Webbook
hfpiz	918.80 ± 5.00	kJ/mol	NIST Webbook
hfus	9.61	kJ/mol	Joback Method
hvap	33.31	kJ/mol	Joback Method
ie	7.43 ± 0.06	eV	NIST Webbook
ie	7.24	eV	NIST Webbook
ie	7.50 ± 0.10	eV	NIST Webbook
ie	7.63	eV	NIST Webbook
ie	7.27 ± 0.03	eV	NIST Webbook
ie	7.20 ± 0.02	eV	NIST Webbook
ie	7.25 ± 0.00	eV	NIST Webbook
ie	7.20	eV	NIST Webbook
ie	7.25 ± 0.00	eV	NIST Webbook
ie	7.24 ± 0.01	eV	NIST Webbook
ie	7.76 ± 0.08	eV	NIST Webbook
log10ws	-1.57		Crippen Method

logp	1.869		Crippen Method
mcvol	83.580	ml/mol	McGowan Method
pc	4356.87	kPa	Joback Method
tb	385.54	K	Joback Method
tc	593.05	K	Joback Method
tf	211.44	K	Joback Method
vc	0.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.68	J/mol×K	385.54	Joback Method
cpg	143.52	J/mol×K	420.12	Joback Method
cpg	153.56	J/mol×K	454.71	Joback Method
cpg	162.85	J/mol×K	489.29	Joback Method
cpg	171.44	J/mol×K	523.88	Joback Method
cpg	179.38	J/mol×K	558.46	Joback Method
cpg	186.73	J/mol×K	593.05	Joback Method
dvisc	0.0010170	Pa×s	211.44	Joback Method
dvisc	0.0007435	Pa×s	240.46	Joback Method
dvisc	0.0005815	Pa×s	269.47	Joback Method
dvisc	0.0004770	Pa×s	298.49	Joback Method
dvisc	0.0004053	Pa×s	327.51	Joback Method
dvisc	0.0003536	Pa×s	356.52	Joback Method
dvisc	0.0003150	Pa×s	385.54	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=C2154565&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfpi:	Enthalpy of formation of positive ion at standard conditions
hfpiz:	Enthalpy of formation of positive ion at 0K
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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