1-Phenylethyl radical

Inchi: InChI=1S/C8H9/c1-2-8-6-4-3-5-7-8/h2-7H,1H3
InchiKey: OGOPVNZBIWLOIJ-UHFFFAOYSA-N
Formula: C8H9
SMILES: C[CH]c1ccccc1
Mol. weight [g/mol]: 105.16
CAS: 2348-51-8

Physical Properties

Property code	Value	Unit	Source
affp	836.50	kJ/mol	NIST Webbook
basg	804.00	kJ/mol	NIST Webbook
ea	0.84 ± 0.11	eV	NIST Webbook
gf	178.83	kJ/mol	Joback Method
hf	78.61	kJ/mol	Joback Method
hfus	8.68	kJ/mol	Joback Method
hvap	35.14	kJ/mol	Joback Method
ie	6.90	eV	NIST Webbook
log10ws	-1.99		Crippen Method
logp	2.259		Crippen Method
mcvol	97.670	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
tb	407.98	K	Joback Method
tc	618.68	K	Joback Method
tf	207.71	K	Joback Method
vc	0.360	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.58	J/mol×K	407.98	Joback Method
cpg	223.72	J/mol×K	583.56	Joback Method
cpg	214.46	J/mol×K	548.45	Joback Method
cpg	204.47	J/mol×K	513.33	Joback Method
cpg	193.70	J/mol×K	478.21	Joback Method

cpg	182.09	J/mol×K	443.10	Joback Method
cpg	232.31	J/mol×K	618.68	Joback Method
dvisc	0.0003329	Pa×s	407.98	Joback Method
dvisc	0.0003862	Pa×s	374.60	Joback Method
dvisc	0.0004614	Pa×s	341.22	Joback Method
dvisc	0.0005728	Pa×s	307.85	Joback Method
dvisc	0.0007496	Pa×s	274.47	Joback Method
dvisc	0.0010568	Pa×s	241.09	Joback Method
dvisc	0.0016637	Pa×s	207.71	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=C2348518&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
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