Isopropyl radical

Inchi: InChI=1S/C3H7/c1-3-2/h3H,1-2H3
InchiKey: HNUALPPJLMYHDK-UHFFFAOYSA-N
Formula: C3H7
SMILES: C[CH]C
Mol. weight [g/mol]: 43.09
CAS: 2025-55-0

Physical Properties

Property code	Value	Unit	Source
affp	671.40	kJ/mol	NIST Webbook
basg	638.90	kJ/mol	NIST Webbook
ea	-0.32 ± 0.09	eV	NIST Webbook
ea	0.69	eV	NIST Webbook
gf	24.32	kJ/mol	Joback Method
hf	90.00 ± 2.00	kJ/mol	NIST Webbook
hfpi	801.00 ± 4.00	kJ/mol	NIST Webbook
hfpiz	818.00 ± 4.00	kJ/mol	NIST Webbook
hfus	1.69	kJ/mol	Joback Method
hvap	21.74	kJ/mol	Joback Method
ie	7.36 ± 0.02	eV	NIST Webbook
ie	7.55	eV	NIST Webbook
ie	7.55 ± 0.05	eV	NIST Webbook
ie	7.37 ± 0.02	eV	NIST Webbook
ie	7.50 ± 0.10	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
ie	7.67 ± 0.02	eV	NIST Webbook
ie	7.57 ± 0.05	eV	NIST Webbook
log10ws	-0.69		Crippen Method
logp	1.230		Crippen Method
mcvol	50.980	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
tb	266.90	K	Joback Method
tc	427.01	K	Joback Method
tf	124.94	K	Joback Method
vc	0.189	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	61.84	J/mol×K	266.90	Joback Method
cpg	89.75	J/mol×K	400.32	Joback Method
cpg	84.77	J/mol×K	373.64	Joback Method
cpg	79.51	J/mol×K	346.95	Joback Method
cpg	73.94	J/mol×K	320.27	Joback Method
cpg	68.06	J/mol×K	293.58	Joback Method
cpg	94.46	J/mol×K	427.01	Joback Method
dvisc	0.0001200	Pa×s	266.90	Joback Method
dvisc	0.0001280	Pa×s	243.24	Joback Method
dvisc	0.0001384	Pa×s	219.58	Joback Method
dvisc	0.0001525	Pa×s	195.92	Joback Method
dvisc	0.0001726	Pa×s	172.26	Joback Method
dvisc	0.0002032	Pa×s	148.60	Joback Method
dvisc	0.0002545	Pa×s	124.94	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=C2025550&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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