n-Propyl radical

Inchi: InChI=1S/C3H7/c1-3-2/h1,3H2,2H3
InchiKey: OCBFFGCSTGGPSQ-UHFFFAOYSA-N
Formula: C3H7
SMILES: [CH2]CC
Mol. weight [g/mol]: 43.09
CAS: 2143-61-5

Physical Properties

Property code	Value	Unit	Source
ea	-0.07 ± 0.12	eV	NIST Webbook
gf	26.76	kJ/mol	Joback Method
hf	100.00 ± 2.00	kJ/mol	NIST Webbook
hfus	5.21	kJ/mol	Joback Method
hvap	22.12	kJ/mol	Joback Method
ie	8.09 ± 0.01	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	8.20 ± 0.10	eV	NIST Webbook
ie	8.13 ± 0.05	eV	NIST Webbook
ie	8.10 ± 0.05	eV	NIST Webbook
ie	8.35 ± 0.01	eV	NIST Webbook
ie	8.15 ± 0.02	eV	NIST Webbook
ie	8.43 ± 0.02	eV	NIST Webbook
log10ws	-0.69		Crippen Method
logp	1.230		Crippen Method
mcvol	50.980	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
tb	267.34	K	Joback Method
tc	423.42	K	Joback Method
tf	139.94	K	Joback Method
vc	0.195	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	62.29	J/mol×K	267.34	Joback Method
cpg	68.24	J/mol×K	293.35	Joback Method
cpg	73.88	J/mol×K	319.37	Joback Method
cpg	79.23	J/mol×K	345.38	Joback Method
cpg	84.29	J/mol×K	371.39	Joback Method
cpg	89.09	J/mol×K	397.40	Joback Method
cpg	93.63	J/mol×K	423.42	Joback Method
dvisc	0.0001909	Pa×s	139.94	Joback Method
dvisc	0.0001675	Pa×s	161.17	Joback Method
dvisc	0.0001515	Pa×s	182.41	Joback Method
dvisc	0.0001400	Pa×s	203.64	Joback Method
dvisc	0.0001312	Pa×s	224.87	Joback Method
dvisc	0.0001244	Pa×s	246.11	Joback Method
dvisc	0.0001190	Pa×s	267.34	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2143615&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
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