

Neopentyl radical

Inchi: InChI=1S/C5H11/c1-5(2,3)4/h1H2,2-4H3
InchiKey: GJWHXWMUGWZNT0-UHFFFAOYSA-N
Formula: C5H11
SMILES: [CH2]C(C)(C)C
Mol. weight [g/mol]: 71.14
CAS: 3744-21-6

Physical Properties

Property code	Value	Unit	Source
gf	46.44	kJ/mol	Joback Method
hf	-99.47	kJ/mol	Joback Method
hfus	2.97	kJ/mol	Joback Method
hvap	25.28	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.867		Crippen Method
mcvol	79.160	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
tb	309.87	K	Joback Method
tc	480.48	K	Joback Method
tf	164.90	K	Joback Method
vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	119.34	J/mol×K	309.87	Joback Method
cpg	129.95	J/mol×K	338.31	Joback Method
cpg	139.93	J/mol×K	366.74	Joback Method
cpg	149.29	J/mol×K	395.18	Joback Method
cpg	158.08	J/mol×K	423.61	Joback Method
cpg	166.33	J/mol×K	452.05	Joback Method
cpg	174.06	J/mol×K	480.48	Joback Method
dvisc	0.0014388	Pa×s	164.90	Joback Method
dvisc	0.0009267	Pa×s	189.06	Joback Method

dvisc	0.0006595	Pa×s	213.22	Joback Method
dvisc	0.0005029	Pa×s	237.38	Joback Method
dvisc	0.0004033	Pa×s	261.55	Joback Method
dvisc	0.0003356	Pa×s	285.71	Joback Method
dvisc	0.0002875	Pa×s	309.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3744216&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
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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