

Heptyl peroxy radical

Inchi:	InChI=1S/C7H15O2/c1-2-3-4-5-6-7-9-8/h2-7H2,1H3
InchiKey:	UHYPWESTSMPXTM-UHFFFAOYSA-N
Formula:	C7H15O2
SMILES:	CCCCCCCO[O]
Mol. weight [g/mol]:	131.19
CAS:	20682-80-8

Physical Properties

Property code	Value	Unit	Source
gf	-249.93	kJ/mol	Joback Method
hf	-449.28	kJ/mol	Joback Method
hfus	19.94	kJ/mol	Joback Method
hvap	38.44	kJ/mol	Joback Method
ie	8.30 ± 0.20	eV	NIST Webbook
log10ws	-6.72		Crippen Method
logp	2.319		Crippen Method
mcvol	119.080	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
tb	417.08	K	Joback Method
tc	586.89	K	Joback Method
tf	227.35	K	Joback Method
vc	0.445	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.86	J/mol×K	417.08	Joback Method
cpg	277.05	J/mol×K	558.59	Joback Method
cpg	268.13	J/mol×K	530.29	Joback Method
cpg	258.76	J/mol×K	501.99	Joback Method
cpg	248.94	J/mol×K	473.68	Joback Method
cpg	238.65	J/mol×K	445.38	Joback Method
cpg	285.56	J/mol×K	586.89	Joback Method
dvisc	0.0003956	Paxs	417.08	Joback Method

dvisc	0.0004727	Paxs	385.46	Joback Method
dvisc	0.0005831	Paxs	353.84	Joback Method
dvisc	0.0007495	Paxs	322.21	Joback Method
dvisc	0.0010174	Paxs	290.59	Joback Method
dvisc	0.0014883	Paxs	258.97	Joback Method
dvisc	0.0024199	Paxs	227.35	Joback Method

Sources

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=C20682808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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