

2-Heptyl radical

Inchi:	InChI=1S/C7H15/c1-3-5-7-6-4-2/h3H,4-7H2,1-2H3
InchiKey:	DOEYHYKYGYGBRH-UHFFFAOYSA-N
Formula:	C7H15
SMILES:	C[CH]CCCCC
Mol. weight [g/mol]:	99.19
CAS:	3474-30-4

Physical Properties

Property code	Value	Unit	Source
gf	58.00	kJ/mol	Joback Method
hf	-137.28	kJ/mol	Joback Method
hfus	12.04	kJ/mol	Joback Method
hvap	30.64	kJ/mol	Joback Method
ie	6.95	eV	NIST Webbook
ie	7.35 ± 0.06	eV	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.791		Crippen Method
mcvol	107.340	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
tb	358.42	K	Joback Method
tc	522.82	K	Joback Method
tf	170.02	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.61	J/molxK	358.42	Joback Method
cpg	200.40	J/molxK	385.82	Joback Method
cpg	211.65	J/molxK	413.22	Joback Method
cpg	222.38	J/molxK	440.62	Joback Method
cpg	232.62	J/molxK	468.02	Joback Method
cpg	242.39	J/molxK	495.42	Joback Method
cpg	251.71	J/molxK	522.82	Joback Method

dvisc	0.0016651	Paxs	170.02	Joback Method
dvisc	0.0010026	Paxs	201.42	Joback Method
dvisc	0.0006922	Paxs	232.82	Joback Method
dvisc	0.0005219	Paxs	264.22	Joback Method
dvisc	0.0004178	Paxs	295.62	Joback Method
dvisc	0.0003491	Paxs	327.02	Joback Method
dvisc	0.0003010	Paxs	358.42	Joback Method

Sources

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=C3474304&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
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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