

Nonane, 5-methylene-

Other names:	1-Hexene, 2-butyl- 2-Butyl-1-hexene 5-Methylenenonane
Inchi:	InChI=1S/C10H20/c1-4-6-8-10(3)9-7-5-2/h3-9H2,1-2H3
InchiKey:	SEFXBCYTMUNYFC-UHFFFAOYSA-N
Formula:	C10H20
SMILES:	C=C(CCCC)CCCC
Mol. weight [g/mol]:	140.27
CAS:	6795-79-5

Physical Properties

Property code	Value	Unit	Source
gf	112.61	kJ/mol	Joback Method
hf	-134.09	kJ/mol	Joback Method
hfus	19.07	kJ/mol	Joback Method
hvap	37.26	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.923		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	975.00		NIST Webbook
rinpol	975.00		NIST Webbook
tb	424.76	K	Joback Method
tc	593.45	K	Joback Method
tf	186.74	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.06	J/mol×K	424.76	Joback Method
cpg	313.92	J/mol×K	452.88	Joback Method
cpg	328.19	J/mol×K	480.99	Joback Method
cpg	341.88	J/mol×K	509.11	Joback Method

cpg	355.03	J/mol×K	537.22	Joback Method
cpg	367.63	J/mol×K	565.34	Joback Method
cpg	379.71	J/mol×K	593.45	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=C6795795&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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