4-Nonene, 5-butyl-

Other names: 5-Butyl-4-nonene
5-n-Butyl-4-nonene
Inchi: InChI=1S/C13H26/c1-4-7-10-13(11-8-5-2)12-9-6-3/h10H,4-9,11-12H2,1-3H3
InchiKey: UKAAUKLRJKBIDI-UHFFFAOYSA-N
Formula: C13H26
SMILES: CCCC=C(CCCC)CCCC
Mol. weight [g/mol]: 182.35
CAS: 7367-38-6

Physical Properties

Property code	Value	Unit	Source
gf	130.25	kJ/mol	Joback Method
hf	-204.22	kJ/mol	Joback Method
hfus	28.32	kJ/mol	Joback Method
hvap	44.57	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	5.093		Crippen Method
mcvol	189.730	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
tb	500.88	K	Joback Method
tc	670.61	K	Joback Method
tf	217.23	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.85	J/mol×K	500.88	Joback Method
cpg	456.37	J/mol×K	529.17	Joback Method
cpg	473.16	J/mol×K	557.46	Joback Method
cpg	489.22	J/mol×K	585.75	Joback Method
cpg	504.60	J/mol×K	614.04	Joback Method
cpg	519.32	J/mol×K	642.32	Joback Method
cpg	533.39	J/mol×K	670.61	Joback Method

hvapt	55.80	kJ/mol	335.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42886e+01
Coeff. B	-4.08025e+03
Coeff. C	-7.69950e+01
Temperature range (K), min.	368.42
Temperature range (K), max.	531.51

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7367386&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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

hvapt: Enthalpy of vaporization at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pc: Critical Pressure

pvap: Vapor pressure

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume