

Nonane, 5-butyl-

Other names:	5-Butylnonane 5-n-Butylnonane
Inchi:	InChI=1S/C13H28/c1-4-7-10-13(11-8-5-2)12-9-6-3/h13H,4-12H2,1-3H3
InchiKey:	YXSQPZMAIVSYDV-UHFFFAOYSA-N
Formula:	C13H28
SMILES:	CCCCC(CCCC)CCCC
Mol. weight [g/mol]:	184.36
CAS:	17312-63-9

Physical Properties

Property code	Value	Unit	Source
gf	56.14	kJ/mol	Joback Method
hf	-316.93	kJ/mol	Joback Method
hfus	25.90	kJ/mol	Joback Method
hvap	44.14	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	5.173		Crippen Method
mvol	194.030	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	1204.00		NIST Webbook
tb	496.40	K	Joback Method
tc	659.72	K	Joback Method
tf	221.27	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.59	J/molxK	496.40	Joback Method
cpg	473.45	J/molxK	523.62	Joback Method
cpg	490.62	J/molxK	550.84	Joback Method
cpg	507.13	J/molxK	578.06	Joback Method
cpg	522.98	J/molxK	605.28	Joback Method
cpg	538.20	J/molxK	632.50	Joback Method

cpg	552.81	J/mol×K	659.72	Joback Method
dvisc	0.0096568	Paxs	221.27	Joback Method
dvisc	0.0028515	Paxs	267.12	Joback Method
dvisc	0.0012038	Paxs	312.98	Joback Method
dvisc	0.0006335	Paxs	358.83	Joback Method
dvisc	0.0003856	Paxs	404.69	Joback Method
dvisc	0.0002596	Paxs	450.54	Joback Method
dvisc	0.0001881	Paxs	496.40	Joback Method
hvapt	52.60	kJ/mol	331.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51183e+01
Coeff. B	-4.33751e+03
Coeff. C	-7.75510e+01
Temperature range (K), min.	370.02
Temperature range (K), max.	519.85

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17312639&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/ci9903071
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

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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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