

5-ethyl-5-methylnonane

Inchi:	InChI=1S/C12H26/c1-5-8-10-12(4,7-3)11-9-6-2/h5-11H2,1-4H3
InchiKey:	DZSBQMNPPIKBNF-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CCCCC(C)(CC)CCCC
Mol. weight [g/mol]:	170.33
CAS:	14531-16-9

Physical Properties

Property code	Value	Unit	Source
af	0.4710		Cheméo Relay (1.0)
gf	53.00	kJ/mol	Joback Method
hf	-290.04	kJ/mol	Cheméo Relay (1.0)
hfus	19.42	kJ/mol	Joback Method
hvap	54.57	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.04		Cheméo Relay (1.0)
logp	4.783		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
tb	469.26	K	Cheméo Relay (1.0)
tc	635.91	K	Cheméo Relay (1.0)
tf	184.37	K	Cheméo Relay (1.0)
vc	0.647	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.96	J/mol×K	470.73	Joback Method
cpg	427.03	J/mol×K	499.11	Joback Method
cpg	444.30	J/mol×K	527.48	Joback Method
cpg	460.79	J/mol×K	555.86	Joback Method
cpg	476.54	J/mol×K	584.24	Joback Method
cpg	491.58	J/mol×K	612.61	Joback Method
cpg	505.93	J/mol×K	640.99	Joback Method
dvisc	0.0097058	Pa×s	227.42	Joback Method

dvisc	0.0031716	Pa×s	267.97	Joback Method
dvisc	0.0013906	Pa×s	308.52	Joback Method
dvisc	0.0007385	Pa×s	349.08	Joback Method
dvisc	0.0004474	Pa×s	389.63	Joback Method
dvisc	0.0002979	Pa×s	430.18	Joback Method
dvisc	0.0002128	Pa×s	470.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14531169&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
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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