

Octane, 3-ethyl-4-methyl

Inchi:	InChI=1S/C11H24/c1-5-8-9-10(4)11(6-2)7-3/h10-11H,5-9H2,1-4H3
InchiKey:	LXRSBMFQRZTMNK-UHFFFAOYSA-N
Formula:	C11H24
SMILES:	CCCCC(C)C(CC)CC
Mol. weight [g/mol]:	156.31

Physical Properties

Property code	Value	Unit	Source
gf	36.86	kJ/mol	Joback Method
hf	-280.93	kJ/mol	Joback Method
hfus	17.20	kJ/mol	Joback Method
hvap	39.30	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	4.249		Crippen Method
mcvol	165.850	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpol	1031.00		NIST Webbook
tb	450.20	K	Joback Method
tc	618.81	K	Joback Method
tf	183.73	K	Joback Method
vc	0.639	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.12	J/mol×K	450.20	Joback Method
cpg	376.92	J/mol×K	478.30	Joback Method
cpg	393.08	J/mol×K	506.40	Joback Method
cpg	408.60	J/mol×K	534.51	Joback Method
cpg	423.51	J/mol×K	562.61	Joback Method
cpg	437.81	J/mol×K	590.71	Joback Method
cpg	451.53	J/mol×K	618.81	Joback Method
dvisc	0.0200727	Paxs	183.73	Joback Method
dvisc	0.0044499	Paxs	228.14	Joback Method

dvisc	0.0016118	Paxs	272.55	Joback Method
dvisc	0.0007760	Paxs	316.96	Joback Method
dvisc	0.0004471	Paxs	361.38	Joback Method
dvisc	0.0002907	Paxs	405.79	Joback Method
dvisc	0.0002057	Paxs	450.20	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=R9526&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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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