Octane, 4-ethyl-3-methyl

Inchi: InChI=1S/C11H24/c1-5-8-9-11(7-3)10(4)6-2/h10-11H,5-9H2,1-4H3
InchiKey: BTRAURWAFYPYMW-UHFFFAOYSA-N
Formula: C11H24
SMILES: CCCCC(CC)C(C)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	1017.00		NIST Webbook
tb	450.20	K	Joback Method
tc	618.81	K	Joback Method
tf	183.73	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.12	J/mol×K	450.20	Joback Method
cpg	437.81	J/mol×K	590.71	Joback Method
cpg	423.51	J/mol×K	562.61	Joback Method
cpg	408.60	J/mol×K	534.51	Joback Method
cpg	393.08	J/mol×K	506.40	Joback Method
cpg	376.92	J/mol×K	478.30	Joback Method
cpg	451.53	J/mol×K	618.81	Joback Method
dvisc	0.0002057	Pa×s	450.20	Joback Method
dvisc	0.0002907	Pa×s	405.79	Joback Method

dvisc	0.0004471	Pa×s	361.38	Joback Method
dvisc	0.0007760	Pa×s	316.96	Joback Method
dvisc	0.0016118	Pa×s	272.55	Joback Method
dvisc	0.0044499	Pa×s	228.14	Joback Method
dvisc	0.0200727	Pa×s	183.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R9539&Units=SI
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
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
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