

Decane, 4-ethyl-

Other names:	4-ethyl-decane
Inchi:	InChI=1S/C12H26/c1-4-7-8-9-11-12(6-3)10-5-2/h12H,4-11H2,1-3H3
InchiKey:	IGTKVLJTIZALGL-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CCCCCCC(CC)CCC
Mol. weight [g/mol]:	170.33
CAS:	1636-44-8

Physical Properties

Property code	Value	Unit	Source
gf	47.72	kJ/mol	Joback Method
hf	-296.29	kJ/mol	Joback Method
hfus	23.31	kJ/mol	Joback Method
hvap	41.92	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.783		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	1135.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1147.00		NIST Webbook
tb	473.52	K	Joback Method
tc	637.74	K	Joback Method
tf	210.00	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.90	J/mol×K	473.52	Joback Method
cpg	424.06	J/mol×K	500.89	Joback Method
cpg	440.58	J/mol×K	528.26	Joback Method
cpg	456.45	J/mol×K	555.63	Joback Method
cpg	471.71	J/mol×K	583.00	Joback Method

cpg	486.36	J/mol×K	610.37	Joback Method
cpg	500.43	J/mol×K	637.74	Joback Method
dvisc	0.0101808	Pa×s	210.00	Joback Method
dvisc	0.0030132	Pa×s	253.92	Joback Method
dvisc	0.0012770	Pa×s	297.84	Joback Method
dvisc	0.0006749	Pa×s	341.76	Joback Method
dvisc	0.0004124	Pa×s	385.68	Joback Method
dvisc	0.0002787	Pa×s	429.60	Joback Method
dvisc	0.0002026	Pa×s	473.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1636448&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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