

Decane, 3,4-dimethyl-

Other names:	3,4-Dimethyl decane
Inchi:	InChI=1S/C12H26/c1-5-7-8-9-10-12(4)11(3)6-2/h11-12H,5-10H2,1-4H3
InchiKey:	NRBMEEEDORZDRIT-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CCCCCCC(C)C(C)CC
Mol. weight [g/mol]:	170.33
CAS:	17312-45-7

Physical Properties

Property code	Value	Unit	Source
gf	45.28	kJ/mol	Joback Method
hf	-301.57	kJ/mol	Joback Method
hfus	19.79	kJ/mol	Joback Method
hvap	41.53	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.639		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
tb	473.08	K	Joback Method
tc	640.63	K	Joback Method
tf	195.00	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.97	J/molxK	473.08	Joback Method
cpg	488.21	J/molxK	612.70	Joback Method
cpg	473.26	J/molxK	584.78	Joback Method
cpg	457.68	J/molxK	556.85	Joback Method
cpg	441.45	J/molxK	528.93	Joback Method
cpg	424.55	J/molxK	501.00	Joback Method
cpg	502.54	J/molxK	640.63	Joback Method
dvisc	0.0001925	Paxs	473.08	Joback Method

dvisc	0.0002726	Paxs	426.73	Joback Method
dvisc	0.0004202	Paxs	380.39	Joback Method
dvisc	0.0007305	Paxs	334.04	Joback Method
dvisc	0.0015175	Paxs	287.69	Joback Method
dvisc	0.0041744	Paxs	241.35	Joback Method
dvisc	0.0185767	Paxs	195.00	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=C17312457&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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