Undecane, 3,5-dimethyl-

Other names: 3,5-Dimethylundecane
Inchi: InChI=1S/C13H28/c1-5-7-8-9-10-13(4)11-12(3)6-2/h12-13H,5-11H2,1-4H3
InchiKey: YSUJWFQMTUVXNQ-UHFFFAOYSA-N
Formula: C13H28
SMILES: CCCCCCC(C)CC(C)CC
Mol. weight [g/mol]: 184.36
CAS: 17312-81-1

Physical Properties

Property code	Value	Unit	Source
gf	53.70	kJ/mol	Joback Method
hf	-322.21	kJ/mol	Joback Method
hfus	22.38	kJ/mol	Joback Method
hvap	43.76	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	5.029		Crippen Method
mcvol	194.030	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	1223.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1210.70		NIST Webbook
rinpol	1207.20		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1207.00		NIST Webbook
tb	495.96	K	Joback Method
tc	662.44	K	Joback Method
tf	206.27	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.70	J/mol×K	495.96	Joback Method
cpg	540.06	J/mol×K	634.69	Joback Method
cpg	524.55	J/mol×K	606.95	Joback Method
cpg	508.38	J/mol×K	579.20	Joback Method
cpg	491.53	J/mol×K	551.45	Joback Method
cpg	473.97	J/mol×K	523.71	Joback Method
cpg	554.93	J/mol×K	662.44	Joback Method
dvisc	0.0001780	Pa×s	495.96	Joback Method
dvisc	0.0002527	Pa×s	447.68	Joback Method
dvisc	0.0003903	Pa×s	399.40	Joback Method
dvisc	0.0006795	Pa×s	351.12	Joback Method
dvisc	0.0014115	Pa×s	302.83	Joback Method
dvisc	0.0038696	Pa×s	254.55	Joback Method
dvisc	0.0170093	Pa×s	206.27	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17312811&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