Undecane, 6,6-dimethyl-

Other names: 6,6-Dimethylundecane
Inchi: InChI=1S/C13H28/c1-5-7-9-11-13(3,4)12-10-8-6-2/h5-12H2,1-4H3
InchiKey: ZFOODCBUKSMZBZ-UHFFFAOYSA-N
Formula: C13H28
SMILES: CCCCCC(C)(C)CCCCC
Mol. weight [g/mol]: 184.36
CAS: 17312-76-4

Physical Properties

Property code	Value	Unit	Source
gf	61.42	kJ/mol	Joback Method
hf	-320.40	kJ/mol	Joback Method
hfus	22.01	kJ/mol	Joback Method
hvap	43.24	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	5.173		Crippen Method
mcvol	194.030	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	1204.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1200.00		NIST Webbook
tb	493.61	K	Joback Method
tc	662.67	K	Joback Method
tf	238.69	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.75	J/mol×K	493.61	Joback Method
cpg	476.43	J/mol×K	521.79	Joback Method
cpg	494.29	J/mol×K	549.96	Joback Method
cpg	511.35	J/mol×K	578.14	Joback Method

cpg	527.65	J/mol×K	606.32	Joback Method
cpg	543.21	J/mol×K	634.50	Joback Method
cpg	558.07	J/mol×K	662.67	Joback Method
dvisc	0.0090102	Pa×s	238.69	Joback Method
dvisc	0.0029290	Pa×s	281.18	Joback Method
dvisc	0.0012789	Pa×s	323.66	Joback Method
dvisc	0.0006768	Pa×s	366.15	Joback Method
dvisc	0.0004088	Pa×s	408.64	Joback Method
dvisc	0.0002716	Pa×s	451.12	Joback Method
dvisc	0.0001935	Pa×s	493.61	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=C17312764&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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