Undecane, 3,8-dimethyl-

Other names: 3,8-Dimethylundecane
Inchi: InChI=1S/C13H28/c1-5-9-13(4)11-8-7-10-12(3)6-2/h12-13H,5-11H2,1-4H3
InchiKey: WOGVWUCXENBLIV-UHFFFAOYSA-N
Formula: C13H28
SMILES: CCCC(C)CCCCC(C)CC
Mol. weight [g/mol]: 184.36
CAS: 17301-30-3

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	1227.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1228.00		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

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=C17301303&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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