1-ethyl-2-methyl Cyclododecane

Inchi: InChI=1S/C15H30/c1-3-15-13-11-9-7-5-4-6-8-10-12-14(15)2/h14-15H,3-13H2,1-2H3
InchiKey: IGEBPPWLYTWODA-UHFFFAOYSA-N
Formula: C15H30
SMILES: CCC1CCCCCCCCCCC1C
Mol. weight [g/mol]: 210.40

Physical Properties

Property code	Value	Unit	Source
gf	19.56	kJ/mol	Joback Method
hf	-355.91	kJ/mol	Joback Method
hfus	14.91	kJ/mol	Joback Method
hvap	50.14	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.563		Crippen Method
mcvol	211.350	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	1488.00		NIST Webbook
rinpol	1488.00		NIST Webbook
tb	583.10	K	Joback Method
tc	809.77	K	Joback Method
tf	240.83	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.69	J/mol×K	583.10	Joback Method
cpg	695.66	J/mol×K	771.99	Joback Method
cpg	672.91	J/mol×K	734.21	Joback Method
cpg	648.43	J/mol×K	696.43	Joback Method
cpg	622.22	J/mol×K	658.66	Joback Method
cpg	594.31	J/mol×K	620.88	Joback Method
cpg	716.66	J/mol×K	809.77	Joback Method
dvisc	0.0000441	Pa×s	583.10	Joback Method

dvisc	0.0000753	Pa×s	526.06	Joback Method
dvisc	0.0001466	Pa×s	469.01	Joback Method
dvisc	0.0003429	Pa×s	411.97	Joback Method
dvisc	0.0010547	Pa×s	354.92	Joback Method
dvisc	0.0049882	Pa×s	297.88	Joback Method
dvisc	0.0492514	Pa×s	240.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R333950&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