

Cyclopentane, 1-butyl-2-ethyl-

Inchi:	InChI=1S/C11H22/c1-3-5-7-11-9-6-8-10(11)4-2/h10-11H,3-9H2,1-2H3
InchiKey:	YJMFUCKUZMNZLY-UHFFFAOYSA-N
Formula:	C11H22
SMILES:	CCCCC1CCCC1CC
Mol. weight [g/mol]:	154.29
CAS:	72993-32-9

Physical Properties

Property code	Value	Unit	Source
gf	70.58	kJ/mol	Joback Method
hf	-230.23	kJ/mol	Joback Method
hfus	19.25	kJ/mol	Joback Method
hvap	40.03	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	4.003		Crippen Method
mcvol	154.990	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	1083.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1087.00		NIST Webbook
tb	461.69	K	Joback Method
tc	648.77	K	Joback Method
tf	220.39	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.22	J/molxK	461.69	Joback Method
cpg	435.30	J/molxK	617.59	Joback Method
cpg	419.15	J/molxK	586.41	Joback Method
cpg	402.19	J/molxK	555.23	Joback Method

cpg	384.40	J/molxK	524.05	Joback Method
cpg	365.75	J/molxK	492.87	Joback Method
cpg	450.67	J/molxK	648.77	Joback Method
dvisc	0.0003027	Paxs	461.69	Joback Method
dvisc	0.0003729	Paxs	421.47	Joback Method
dvisc	0.0004801	Paxs	381.26	Joback Method
dvisc	0.0006560	Paxs	341.04	Joback Method
dvisc	0.0009745	Paxs	300.82	Joback Method
dvisc	0.0016355	Paxs	260.61	Joback Method
dvisc	0.0033159	Paxs	220.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72993329&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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