

1-trans-2-Ethylmethylcyclopentane

Inchi:	InChI=1S/C8H16/c1-3-8-6-4-5-7(8)2/h7-8H,3-6H2,1-2H3/t7-,8-/m1/s1
InchiKey:	BSKOLJVTLRLTHE-HTQZYQBOSA-N
Formula:	C8H16
SMILES:	CCC1CCCC1C
Mol. weight [g/mol]:	112.21

Physical Properties

Property code	Value	Unit	Source
gf	45.32	kJ/mol	Joback Method
hf	-168.31	kJ/mol	Joback Method
hfus	11.48	kJ/mol	Joback Method
hvap	33.35	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	787.00		NIST Webbook
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tb	393.05	K	Joback Method
tc	585.20	K	Joback Method
tf	186.58	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.75	J/mol×K	393.05	Joback Method
cpg	230.45	J/mol×K	425.08	Joback Method
cpg	246.41	J/mol×K	457.10	Joback Method
cpg	261.64	J/mol×K	489.13	Joback Method
cpg	276.17	J/mol×K	521.15	Joback Method
cpg	290.01	J/mol×K	553.18	Joback Method
cpg	303.19	J/mol×K	585.20	Joback Method
dvisc	0.0022106	Pa×s	186.58	Joback Method

dvisc	0.0012051	Pa×s	220.99	Joback Method
dvisc	0.0007737	Pa×s	255.40	Joback Method
dvisc	0.0005518	Pa×s	289.81	Joback Method
dvisc	0.0004228	Pa×s	324.23	Joback Method
dvisc	0.0003410	Pa×s	358.64	Joback Method
dvisc	0.0002855	Pa×s	393.05	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R633928&Units=SI

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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