trans-1,2-Diethyl cyclopentane

Other names: Cyclopentane, 1,2-diethyl-, trans-
Inchi: InChI=1S/C9H18/c1-3-8-6-5-7-9(8)4-2/h8-9H,3-7H2,1-2H3/t8-,9-/m0/s1
InchiKey: JKMYLSLBFNMSFP-IUCAKERBSA-N
Formula: C9H18
SMILES: CCC1CCCC1CC
Mol. weight [g/mol]: 126.24
CAS: 932-40-1

Physical Properties

Property code	Value	Unit	Source
gf	53.74	kJ/mol	Joback Method
hf	-188.95	kJ/mol	Joback Method
hfus	14.07	kJ/mol	Joback Method
hvap	35.58	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	888.80		NIST Webbook
rinpol	892.50		NIST Webbook
rinpol	888.80		NIST Webbook
tb	421.63 ± 0.60	K	NIST Webbook
tc	606.59	K	Joback Method
tf	177.60 ± 1.00	K	NIST Webbook
tf	177.60 ± 1.00	K	NIST Webbook
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.81	J/mol×K	415.93	Joback Method
cpg	273.59	J/mol×K	447.71	Joback Method
cpg	290.58	J/mol×K	479.48	Joback Method
cpg	306.79	J/mol×K	511.26	Joback Method

cpg	322.25	J/mol×K	543.03	Joback Method
cpg	336.97	J/mol×K	574.81	Joback Method
cpg	350.98	J/mol×K	606.59	Joback Method
dvisc	0.0026275	Pa×s	197.85	Joback Method
dvisc	0.0013798	Pa×s	234.20	Joback Method
dvisc	0.0008615	Pa×s	270.54	Joback Method
dvisc	0.0006014	Pa×s	306.89	Joback Method
dvisc	0.0004530	Pa×s	343.24	Joback Method
dvisc	0.0003603	Pa×s	379.58	Joback Method
dvisc	0.0002982	Pa×s	415.93	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C932401&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

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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