

trans-1,3-Diethylcyclopentane

Inchi:	InChI=1S/C9H18/c1-3-8-5-6-9(4-2)7-8/h8-9H,3-7H2,1-2H3/t8-,9-/m0/s1
InchiKey:	RUUVWUNHERVOAY-IUCAKERBSA-N
Formula:	C9H18
SMILES:	CCC1CCC(CC)C1
Mol. weight [g/mol]:	126.24

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	895.40		NIST Webbook
rinpol	899.00		NIST Webbook
tb	415.93	K	Joback Method
tc	606.59	K	Joback Method
tf	197.85	K	Joback Method
vc	0.479	m ³ /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	Paxs	197.85	Joback Method

dvisc	0.0013798	Paxs	234.20	Joback Method
dvisc	0.0008615	Paxs	270.54	Joback Method
dvisc	0.0006014	Paxs	306.89	Joback Method
dvisc	0.0004530	Paxs	343.24	Joback Method
dvisc	0.0003603	Paxs	379.58	Joback Method
dvisc	0.0002982	Paxs	415.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=522
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U113871&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
mvol:	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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