trans-1-Ethyl-3-methylcyclohexane

Other names: 1-Ethyl-3-methylcyclohexane, trans
Inchi: InChI=1S/C9H18/c1-3-9-6-4-5-8(2)7-9/h8-9H,3-7H2,1-2H3/t8-,9-/m0/s1
InchiKey: UDDVMPHNQKRNNS-IUCAKERBSA-N
Formula: C9H18
SMILES: CCC1CCCC(C)C1
Mol. weight [g/mol]: 126.24
CAS: 4926-76-5

Physical Properties

Property code	Value	Unit	Source
gf	41.64	kJ/mol	Joback Method
hf	-195.11	kJ/mol	Joback Method
hfus	11.97	kJ/mol	Joback Method
hvap	35.75	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	908.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	926.00		NIST Webbook
tb	421.70 ± 2.00	K	NIST Webbook
tb	421.70 ± 2.00	K	NIST Webbook
tb	421.70 ± 1.00	K	NIST Webbook
tb	421.70 ± 1.00	K	NIST Webbook
tc	618.70	K	Joback Method
tf	194.33	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.07	J/mol×K	420.20	Joback Method
cpg	340.98	J/mol×K	585.62	Joback Method
cpg	325.42	J/mol×K	552.53	Joback Method
cpg	309.07	J/mol×K	519.45	Joback Method
cpg	291.90	J/mol×K	486.37	Joback Method
cpg	273.91	J/mol×K	453.28	Joback Method
cpg	355.76	J/mol×K	618.70	Joback Method
dvisc	0.0002668	Pa×s	420.20	Joback Method
dvisc	0.0003400	Pa×s	382.56	Joback Method
dvisc	0.0004567	Pa×s	344.91	Joback Method
dvisc	0.0006594	Pa×s	307.26	Joback Method
dvisc	0.0010552	Pa×s	269.62	Joback Method
dvisc	0.0019666	Pa×s	231.97	Joback Method
dvisc	0.0046654	Pa×s	194.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4926765&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

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