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-/m1/s1
InchiKey: UDDVMPHNQKRNNS-IUCAKERBSA-N
Formula: C9H18
SMILES: CC[C@@H]1CCC[C@@H](C)C1
Mol. weight [g/mol]: 126.24

Physical Properties

Property code	Value	Unit	Source
af	0.2295		Cheméo Relay (1.0)
gf	41.64	kJ/mol	Joback Method
hf	-192.92	kJ/mol	Cheméo Relay (1.0)
hfus	11.97	kJ/mol	Joback Method
hvap	40.66	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	Cheméo Relay (1.0)
log10ws	-4.90		Cheméo Relay (1.0)
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	911.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	908.00		NIST Webbook
tb	421.70 ± 2.00	K	NIST Webbook
tb	421.70 ± 1.00	K	NIST Webbook
tb	421.70 ± 2.00	K	NIST Webbook
tb	421.70 ± 1.00	K	NIST Webbook
tc	625.44	K	Cheméo Relay (1.0)
tf	166.08	K	Cheméo Relay (1.0)
vc	0.480	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4926765&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
ie:	Ionization energy
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