1-Ethyl-4-methylcyclohexane

Inchi: InChI=1S/C9H18/c1-3-9-6-4-8(2)5-7-9/h8-9H,3-7H2,1-2H3
InchiKey: CYISMTMRBPPERU-UHFFFAOYSA-N
Formula: C9H18
SMILES: CCC1CCC(C)CC1
Mol. weight [g/mol]: 126.24
CAS: 3728-56-1

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	888.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	883.00		NIST Webbook
tb	423.00 ± 4.00	K	NIST Webbook
tb	423.70 ± 2.00	K	NIST Webbook
tb	420.00 ± 3.00	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

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=C3728561&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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