3-Ethyl-5-methyl-1-propyl-cyclohexane

Inchi: InChI=1S/C12H24/c1-4-6-11-8-7-10(3)12(5-2)9-11/h10-12H,4-9H2,1-3H3
InchiKey: HYWLHMWDFMUUEH-UHFFFAOYSA-N
Formula: C12H24
SMILES: CCCC1CCC(C)C(CC)C1
Mol. weight [g/mol]: 168.32

Physical Properties

Property code	Value	Unit	Source
gf	59.19	kJ/mol	Joback Method
hf	-277.37	kJ/mol	Joback Method
hfus	20.81	kJ/mol	Joback Method
hvap	42.12	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	4.249		Crippen Method
mcvol	169.080	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	190.30		NIST Webbook
rinpol	190.30		NIST Webbook
tb	484.17	K	Joback Method
tc	675.86	K	Joback Method
tf	223.90	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.69	J/mol×K	484.17	Joback Method
cpg	416.33	J/mol×K	516.12	Joback Method
cpg	437.01	J/mol×K	548.07	Joback Method
cpg	456.75	J/mol×K	580.01	Joback Method
cpg	475.57	J/mol×K	611.96	Joback Method
cpg	493.49	J/mol×K	643.91	Joback Method
cpg	510.52	J/mol×K	675.86	Joback Method
dvisc	0.0033609	Pa×s	223.90	Joback Method

dvisc	0.0015483	Pa×s	267.28	Joback Method
dvisc	0.0008856	Pa×s	310.66	Joback Method
dvisc	0.0005809	Pa×s	354.03	Joback Method
dvisc	0.0004178	Pa×s	397.41	Joback Method
dvisc	0.0003206	Pa×s	440.79	Joback Method
dvisc	0.0002580	Pa×s	484.17	Joback Method

Sources

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=R516640&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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