Cycloheptane, ethyl-

Other names: ethyl-cycloheptane
Inchi: InChI=1S/C9H18/c1-2-9-7-5-3-4-6-8-9/h9H,2-8H2,1H3
InchiKey: ITZHTNFXLDFAPB-UHFFFAOYSA-N
Formula: C9H18
SMILES: CCC1CCCCCC1
Mol. weight [g/mol]: 126.24
CAS: 13151-55-8

Physical Properties

Property code	Value	Unit	Source
gf	37.25	kJ/mol	Joback Method
hf	-180.93	kJ/mol	Joback Method
hfus	8.80	kJ/mol	Joback Method
hvap	36.23	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.367		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	969.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	973.00		NIST Webbook
tb	437.79 ± 0.20	K	NIST Webbook
tc	636.28	K	Joback Method
tf	154.44 ± 0.20	K	NIST Webbook
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.63	J/mol×K	429.14	Joback Method
cpg	343.75	J/mol×K	601.76	Joback Method
cpg	327.74	J/mol×K	567.23	Joback Method
cpg	310.84	J/mol×K	532.71	Joback Method
cpg	293.03	J/mol×K	498.19	Joback Method

cpg	274.30	J/mol×K	463.66	Joback Method
cpg	358.90	J/mol×K	636.28	Joback Method
dvisc	0.0002402	Pa×s	429.14	Joback Method
dvisc	0.0003404	Pa×s	390.12	Joback Method
dvisc	0.0005212	Pa×s	351.11	Joback Method
dvisc	0.0008877	Pa×s	312.10	Joback Method
dvisc	0.0017602	Pa×s	273.08	Joback Method
dvisc	0.0043855	Pa×s	234.06	Joback Method
dvisc	0.0157420	Pa×s	195.05	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol580.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13151558&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

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