Bicyclo[2.2.1]heptane, 2-ethyl-

Other names: Norbornane, 2-ethyl-
2-Ethylbicyclo[2.2.1]heptane
5-Ethylnorbornane
Inchi: InChI=1S/C9H16/c1-2-8-5-7-3-4-9(8)6-7/h7-9H,2-6H2,1H3
InchiKey: DEMFSGPWYVAINM-UHFFFAOYSA-N
Formula: C9H16
SMILES: CCC1CC2CCC1C2
Mol. weight [g/mol]: 124.22
CAS: 2146-41-0

Physical Properties

Property code	Value	Unit	Source
chl	-5688.00 ± 1.80	kJ/mol	NIST Webbook
gf	126.59	kJ/mol	Joback Method
hf	-109.99	kJ/mol	Joback Method
hfl	-140.30 ± 1.90	kJ/mol	NIST Webbook
hfus	14.31	kJ/mol	Joback Method
hvap	35.32	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.833		Crippen Method
mcvol	115.950	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpol	919.90		NIST Webbook
rinpol	915.90		NIST Webbook
rinpol	919.90		NIST Webbook
ripol	1015.10		NIST Webbook
tb	418.40	K	Joback Method
tc	617.34	K	Joback Method
tf	219.31	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	338.31	J/mol×K	617.34	Joback Method
cpg	324.58	J/mol×K	584.18	Joback Method
cpg	309.99	J/mol×K	551.02	Joback Method
cpg	294.50	J/mol×K	517.87	Joback Method
cpg	278.04	J/mol×K	484.71	Joback Method
cpg	260.57	J/mol×K	451.56	Joback Method
cpg	242.04	J/mol×K	418.40	Joback Method
dvisc	0.0006635	Pa×s	219.31	Joback Method
dvisc	0.0005436	Pa×s	418.40	Joback Method
dvisc	0.0005540	Pa×s	385.22	Joback Method
dvisc	0.0005666	Pa×s	352.04	Joback Method
dvisc	0.0005822	Pa×s	318.86	Joback Method
dvisc	0.0006020	Pa×s	285.67	Joback Method
dvisc	0.0006280	Pa×s	252.49	Joback Method
hvapt	44.40	kJ/mol	372.50	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2146410&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume