

Tricyclo[4.1.0.0(2,7)]heptane

Other names:	Tricyclo[3.1.1.0(6,7)]heptane
Inchi:	InChI=1S/C7H10/c1-2-4-6-5(3-1)7(4)6/h4-7H,1-3H2
InchiKey:	HTEFASNITGSEJD-UHFFFAOYSA-N
Formula:	C7H10
SMILES:	C1CC2C3C(C1)C23
Mol. weight [g/mol]:	94.15
CAS:	287-13-8

Physical Properties

Property code	Value	Unit	Source
gf	206.80	kJ/mol	Joback Method
hf	191.00	kJ/mol	NIST Webbook
hfus	13.56	kJ/mol	Joback Method
hvap	30.26	kJ/mol	Joback Method
ie	8.72	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.662		Crippen Method
mcvol	76.910	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	366.57	K	Joback Method
tc	560.65	K	Joback Method
tf	225.27	K	Joback Method
vc	0.314	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.43	J/mol×K	366.57	Joback Method
cpg	164.06	J/mol×K	398.92	Joback Method
cpg	178.49	J/mol×K	431.26	Joback Method
cpg	191.80	J/mol×K	463.61	Joback Method
cpg	204.06	J/mol×K	495.96	Joback Method
cpg	215.38	J/mol×K	528.30	Joback Method

cpg	225.81	J/molxK	560.65	Joback Method
dvisc	0.0000673	Paxs	225.27	Joback Method
dvisc	0.0001139	Paxs	248.82	Joback Method
dvisc	0.0001760	Paxs	272.37	Joback Method
dvisc	0.0002537	Paxs	295.92	Joback Method
dvisc	0.0003466	Paxs	319.47	Joback Method
dvisc	0.0004537	Paxs	343.02	Joback Method
dvisc	0.0005736	Paxs	366.57	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=C287138&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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