

Tricyclo[4.2.0.0^{2,5}]octane, anti-

Inchi: InChI=1S/C8H12/c1-2-6-5(1)7-3-4-8(6)7/h5-8H,1-4H2/t5-,6+,7+,8-
InchiKey: YTZCZYFFHKYOBJ-SOSBWXJGSA-N
Formula: C8H12
SMILES: C1CC2C1C1CCC21
Mol. weight [g/mol]: 108.18
CAS: 13027-75-3

Physical Properties

Property code	Value	Unit	Source
chl	-5032.00 ± 3.00	kJ/mol	NIST Webbook
gf	203.12	kJ/mol	Joback Method
hf	211.00 ± 3.00	kJ/mol	NIST Webbook
hfl	169.00 ± 3.00	kJ/mol	NIST Webbook
hfus	14.05	kJ/mol	Joback Method
hvap	41.80 ± 1.70	kJ/mol	NIST Webbook
hvap	42.00 ± 2.00	kJ/mol	NIST Webbook
hvap	42.00	kJ/mol	NIST Webbook
ie	9.23	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	2.052		Crippen Method
mvol	91.000	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	393.72	K	Joback Method
tc	594.92	K	Joback Method
tf	233.02	K	Joback Method
vc	0.361	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.89	J/mol×K	393.72	Joback Method
cpg	262.25	J/mol×K	561.38	Joback Method
cpg	249.40	J/mol×K	527.85	Joback Method
cpg	235.52	J/mol×K	494.32	Joback Method

cpg	220.54	J/molxK	460.79	Joback Method
cpg	204.36	J/molxK	427.25	Joback Method
cpg	274.16	J/molxK	594.92	Joback Method
dvisc	0.0008202	Paxs	393.72	Joback Method
dvisc	0.0006884	Paxs	366.94	Joback Method
dvisc	0.0005621	Paxs	340.15	Joback Method
dvisc	0.0004433	Paxs	313.37	Joback Method
dvisc	0.0003344	Paxs	286.59	Joback Method
dvisc	0.0002381	Paxs	259.80	Joback Method
dvisc	0.0001567	Paxs	233.02	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=C13027753&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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