Tricyclo[3.2.1.02,4]octane,(1«alpha»,2«beta»,4«be

Inchi: InChI=1S/C8H12/c1-2-6-3-5(1)7-4-8(6)7/h5-8H,1-4H2/t5-,6-,7-,8+/m1/s1
InchiKey: PSZPCAFRANQPLS-XUTVFYLZSA-N
Formula: C8H12
SMILES: C1CC2CC1C1CC21
Mol. weight [g/mol]: 108.18
CAS: 13377-46-3

Physical Properties

Property code	Value	Unit	Source
gf	203.12	kJ/mol	Joback Method
hf	-4.23	kJ/mol	Joback Method
hfus	14.05	kJ/mol	Joback Method
hvap	32.66	kJ/mol	Joback Method
ie	9.10 ± 0.10	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	2.052		Crippen Method
mcvol	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	m3/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/mol×K	460.79	Joback Method
cpg	204.36	J/mol×K	427.25	Joback Method
cpg	274.16	J/mol×K	594.92	Joback Method

dvisc	0.0008202	Pa×s	393.72	Joback Method
dvisc	0.0006884	Pa×s	366.94	Joback Method
dvisc	0.0005621	Pa×s	340.15	Joback Method
dvisc	0.0004433	Pa×s	313.37	Joback Method
dvisc	0.0003344	Pa×s	286.59	Joback Method
dvisc	0.0002381	Pa×s	259.80	Joback Method
dvisc	0.0001567	Pa×s	233.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13377463&Units=SI
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

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