

Tricyclo[4.2.1.0(2,5)]non-7-ene, 3-(tert-butyl)-

Inchi:	InChI=1S/C13H20/c1-13(2,3)11-7-10-8-4-5-9(6-8)12(10)11/h4-5,8-12H,6-7H2,1-3H3
InchiKey:	ZDFYZSBZKSBECD-UHFFFAOYSA-N
Formula:	C13H20
SMILES:	CC(C)(C)C1CC2C3C=CC(C3)C21
Mol. weight [g/mol]:	176.30

Physical Properties

Property code	Value	Unit	Source
gf	258.21	kJ/mol	Joback Method
hf	-84.90	kJ/mol	Joback Method
hfus	19.78	kJ/mol	Joback Method
hvap	42.65	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.491		Crippen Method
mcvol	157.150	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	1211.00		NIST Webbook
tb	503.65	K	Joback Method
tc	715.57	K	Joback Method
tf	284.79	K	Joback Method
vc	0.608	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.68	J/molxK	503.65	Joback Method
cpg	424.04	J/molxK	538.97	Joback Method
cpg	444.77	J/molxK	574.29	Joback Method
cpg	464.02	J/molxK	609.61	Joback Method
cpg	481.90	J/molxK	644.93	Joback Method
cpg	498.52	J/molxK	680.25	Joback Method
cpg	514.03	J/molxK	715.57	Joback Method
dvisc	0.0010062	Paxs	284.79	Joback Method
dvisc	0.0011632	Paxs	321.27	Joback Method

dvisc	0.0013055	Paxs	357.74	Joback Method
dvisc	0.0014342	Paxs	394.22	Joback Method
dvisc	0.0015508	Paxs	430.70	Joback Method
dvisc	0.0016564	Paxs	467.17	Joback Method
dvisc	0.0017525	Paxs	503.65	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U381696&Units=SI

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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