Tricyclo[3.3.1.13,7]decane, 2-ethyl-

Other names: 2-Ethyladamantane
Inchi: InChI=1S/C12H20/c1-2-12-10-4-8-3-9(6-10)7-11(12)5-8/h8-12H,2-7H2,1H3
InchiKey: LIAWCKFOFPPVGF-UHFFFAOYSA-N
Formula: C12H20
SMILES: CCC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 164.29
CAS: 14451-87-7

Physical Properties

Property code	Value	Unit	Source
gf	204.89	kJ/mol	Joback Method
hf	-119.45	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	41.60	kJ/mol	Joback Method
ie	9.20	eV	NIST Webbook
log10ws	-3.32		Crippen Method
logp	3.469		Crippen Method
mcvol	147.360	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1323.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1280.00		NIST Webbook

rinpol	1284.00		NIST Webbook
rinpol	1299.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1262.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1482.00		NIST Webbook
tb	489.11	K	Joback Method
tc	696.52	K	Joback Method
tf	266.82	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.52	J/mol×K	489.11	Joback Method
cpg	466.74	J/mol×K	661.95	Joback Method
cpg	449.39	J/mol×K	627.38	Joback Method
cpg	430.88	J/mol×K	592.81	Joback Method
cpg	411.12	J/mol×K	558.25	Joback Method
cpg	390.03	J/mol×K	523.68	Joback Method
cpg	483.01	J/mol×K	696.52	Joback Method
dvisc	0.0014315	Pa×s	489.11	Joback Method
dvisc	0.0013411	Pa×s	452.06	Joback Method
dvisc	0.0012419	Pa×s	415.01	Joback Method
dvisc	0.0011329	Pa×s	377.96	Joback Method
dvisc	0.0010129	Pa×s	340.92	Joback Method
dvisc	0.0008813	Pa×s	303.87	Joback Method
dvisc	0.0007378	Pa×s	266.82	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=C14451877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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