t-cyclotridecene

Other names: Cyclotridecene, (E)
Inchi: InChI=1S/C13H24/c1-2-4-6-8-10-12-13-11-9-7-5-3-1/h1-2H,3-13H2/b2-1+
InchiKey: AVHHUCROZGSCGZ-OWOJBTEDSA-N
Formula: C13H24
SMILES: C1=CCCCCCCCCCCC1
Mol. weight [g/mol]: 180.33
CAS: 2484-65-3

Physical Properties

Property code	Value	Unit	Source
gf	36.00	kJ/mol	Joback Method
hf	-222.33	kJ/mol	Joback Method
hfus	6.71	kJ/mol	Joback Method
hvap	46.77	kJ/mol	Joback Method
ie	8.63 ± 0.15	eV	NIST Webbook
log10ws	-5.01		Crippen Method
logp	4.847		Crippen Method
mcvol	178.870	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1379.10		NIST Webbook
rinpol	1379.10		NIST Webbook
tb	550.11	K	Joback Method
tc	797.26	K	Joback Method
tf	224.01	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.00	J/mol×K	550.11	Joback Method
cpg	465.44	J/mol×K	591.30	Joback Method
cpg	492.10	J/mol×K	632.49	Joback Method
cpg	516.97	J/mol×K	673.69	Joback Method
cpg	540.04	J/mol×K	714.88	Joback Method

cpg	561.31	J/mol×K	756.07	Joback Method
cpg	580.75	J/mol×K	797.26	Joback Method
dvisc	0.2372933	Pa×s	224.01	Joback Method
dvisc	0.0133192	Pa×s	278.36	Joback Method
dvisc	0.0019157	Pa×s	332.71	Joback Method
dvisc	0.0004750	Pa×s	387.06	Joback Method
dvisc	0.0001660	Pa×s	441.41	Joback Method
dvisc	0.0000731	Pa×s	495.76	Joback Method
dvisc	0.0000378	Pa×s	550.11	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2484653&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from: