

trans-1-Methoxycyclotridecene

Inchi:	InChI=1S/C14H26O/c1-15-14-12-10-8-6-4-2-3-5-7-9-11-13-14/h12H,2-11,13H2,1H3/b14-
InchiKey:	DQNSWVPJRZTUNF-OWBHPGMISA-N
Formula:	C14H26O
SMILES:	COC1=CCCCCCCCCCC1
Mol. weight [g/mol]:	210.36
CAS:	78289-10-8

Physical Properties

Property code	Value	Unit	Source
gf	-70.21	kJ/mol	Joback Method
hf	-386.66	kJ/mol	Joback Method
hfus	10.10	kJ/mol	Joback Method
hvap	52.06	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.821		Crippen Method
mcvol	198.830	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
tb	600.39	K	Joback Method
tc	839.73	K	Joback Method
tf	270.03	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.64	J/molxK	600.39	Joback Method
cpg	551.00	J/molxK	640.28	Joback Method
cpg	576.65	J/molxK	680.17	Joback Method
cpg	600.57	J/molxK	720.06	Joback Method
cpg	622.72	J/molxK	759.95	Joback Method
cpg	643.06	J/molxK	799.84	Joback Method
cpg	661.56	J/molxK	839.73	Joback Method
dvisc	0.0252648	Paxs	270.03	Joback Method
dvisc	0.0028674	Paxs	325.09	Joback Method

dvisc	0.0006112	Paxs	380.15	Joback Method
dvisc	0.0001927	Paxs	435.21	Joback Method
dvisc	0.0000787	Paxs	490.27	Joback Method
dvisc	0.0000385	Paxs	545.33	Joback Method
dvisc	0.0000215	Paxs	600.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78289108&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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