

trans-1-Methoxycycloundecene

Inchi:	InChI=1S/C12H22O/c1-13-12-10-8-6-4-2-3-5-7-9-11-12/h10H,2-9,11H2,1H3/b12-10-
InchiKey:	ZBQOWEVXPQWKGB-BENRWUELSA-N
Formula:	C12H22O
SMILES:	COC1=CCCCCCCCC1
Mol. weight [g/mol]:	182.30
CAS:	78289-09-5

Physical Properties

Property code	Value	Unit	Source
gf	-62.85	kJ/mol	Joback Method
hf	-333.06	kJ/mol	Joback Method
hfus	9.12	kJ/mol	Joback Method
hvap	47.27	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.041		Crippen Method
mvol	170.650	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
tb	546.09	K	Joback Method
tc	778.11	K	Joback Method
tf	254.53	K	Joback Method
vc	0.606	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.15	J/molxK	546.09	Joback Method
cpg	520.62	J/molxK	739.44	Joback Method
cpg	501.84	J/molxK	700.77	Joback Method
cpg	481.68	J/molxK	662.10	Joback Method
cpg	460.17	J/molxK	623.43	Joback Method
cpg	437.32	J/molxK	584.76	Joback Method
cpg	538.01	J/molxK	778.11	Joback Method
dvisc	0.0000529	Paxs	546.09	Joback Method
dvisc	0.0000882	Paxs	497.50	Joback Method

dvisc	0.0001641	Paxs	448.90	Joback Method
dvisc	0.0003551	Paxs	400.31	Joback Method
dvisc	0.0009509	Paxs	351.72	Joback Method
dvisc	0.0034923	Paxs	303.12	Joback Method
dvisc	0.0210777	Paxs	254.53	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=C78289095&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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