Tricyclo[4.3.1.1(2,5)]undecane, 10-methoxy-, stereoisomer

Inchi: InChI=1S/C12H20O/c1-13-12-10-3-2-4-11(12)9-6-5-8(10)7-9/h8-12H,2-7H2,1H3
InchiKey: FZLYZEQLJWOGIF-UHFFFAOYSA-N
Formula: C12H20O
SMILES: COC1C2CCCC1C1CCC2C1
Mol. weight [g/mol]: 180.29
CAS: 85538-50-7

Physical Properties

Property code	Value	Unit	Source
gf	87.79	kJ/mol	Joback Method
hf	-257.83	kJ/mol	Joback Method
hfus	20.37	kJ/mol	Joback Method
hvap	44.18	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	-2.76		Crippen Method
logp	2.848		Crippen Method
mcvol	153.230	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
tb	515.80	K	Joback Method
tc	729.04	K	Joback Method
tf	285.53	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.11	J/mol×K	515.80	Joback Method
cpg	420.91	J/mol×K	551.34	Joback Method
cpg	442.33	J/mol×K	586.88	Joback Method
cpg	462.43	J/mol×K	622.42	Joback Method
cpg	481.29	J/mol×K	657.96	Joback Method
cpg	498.97	J/mol×K	693.50	Joback Method
cpg	515.56	J/mol×K	729.04	Joback Method

dvisc	0.0010770	Pa×s	285.53	Joback Method
dvisc	0.0011013	Pa×s	323.91	Joback Method
dvisc	0.0011208	Pa×s	362.29	Joback Method
dvisc	0.0011369	Pa×s	400.66	Joback Method
dvisc	0.0011503	Pa×s	439.04	Joback Method
dvisc	0.0011616	Pa×s	477.42	Joback Method
dvisc	0.0011714	Pa×s	515.80	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=C85538507&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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