

trans-1-Methoxycyclododecene

Inchi:	InChI=1S/C13H24O/c1-14-13-11-9-7-5-3-2-4-6-8-10-12-13/h11H,2-10,12H2,1H3/b13-11
InchiKey:	QKXCGPJJHMULFJ-QBFSEMIESA-N
Formula:	C13H24O
SMILES:	COC1=CCCCCCCCCCC1
Mol. weight [g/mol]:	196.33
CAS:	51238-63-2

Physical Properties

Property code	Value	Unit	Source
gf	-66.53	kJ/mol	Joback Method
hf	-359.86	kJ/mol	Joback Method
hfus	9.61	kJ/mol	Joback Method
hvap	49.67	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.431		Crippen Method
mcvol	184.740	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
tb	573.24	K	Joback Method
tc	809.09	K	Joback Method
tf	262.28	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.16	J/molxK	573.24	Joback Method
cpg	493.02	J/molxK	612.55	Joback Method
cpg	517.37	J/molxK	651.86	Joback Method
cpg	540.19	J/molxK	691.17	Joback Method
cpg	561.46	J/molxK	730.47	Joback Method
cpg	581.14	J/molxK	769.78	Joback Method
cpg	599.22	J/molxK	809.09	Joback Method
dvisc	0.0237009	Paxs	262.28	Joback Method
dvisc	0.0032430	Paxs	314.11	Joback Method

dvisc	0.0007795	Paxs	365.93	Joback Method
dvisc	0.0002669	Paxs	417.76	Joback Method
dvisc	0.0001157	Paxs	469.59	Joback Method
dvisc	0.0000593	Paxs	521.41	Joback Method
dvisc	0.0000343	Paxs	573.24	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C51238632&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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