Heptyl tert-pentyl ether

Inchi: InChI=1S/C12H26O/c1-5-7-8-9-10-11-13-12(3,4)6-2/h5-11H2,1-4H3
InchiKey: SHGLLHAAYXCZQW-UHFFFAOYSA-N
Formula: C12H26O
SMILES: CCCCCCCOC(C)(C)CC
Mol. weight [g/mol]: 186.33

Physical Properties

Property code	Value	Unit	Source
gf	-52.00	kJ/mol	Joback Method
hf	-431.98	kJ/mol	Joback Method
hfus	20.61	kJ/mol	Joback Method
hvap	43.42	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	4.162		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1101.00		NIST Webbook
tb	493.15	K	Joback Method
tc	663.06	K	Joback Method
tf	249.65	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.06	J/mol×K	493.15	Joback Method
cpg	455.66	J/mol×K	521.47	Joback Method
cpg	472.52	J/mol×K	549.79	Joback Method
cpg	488.68	J/mol×K	578.11	Joback Method
cpg	504.13	J/mol×K	606.43	Joback Method
cpg	518.92	J/mol×K	634.75	Joback Method
cpg	533.06	J/mol×K	663.06	Joback Method
dvisc	0.0060945	Pa×s	249.65	Joback Method
dvisc	0.0022201	Pa×s	290.23	Joback Method

dvisc	0.0010361	Pa×s	330.82	Joback Method
dvisc	0.0005712	Pa×s	371.40	Joback Method
dvisc	0.0003541	Pa×s	411.98	Joback Method
dvisc	0.0002391	Pa×s	452.57	Joback Method
dvisc	0.0001723	Pa×s	493.15	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=R559721&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
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:
https://www.chemeo.com/cid/61-003-0/Heptyl-tert-pentyl-ether.pdf
Generated by Cheméo on 2024-04-20 13:25:20.261671943 +0000 UTC m=+15908769.182249260.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.