

Octyl tert-butyl ether

Inchi:	InChI=1S/C12H26O/c1-5-6-7-8-9-10-11-13-12(2,3)4/h5-11H2,1-4H3
InchiKey:	DXJWXUJMLBHMHP-UHFFFAOYSA-N
Formula:	C12H26O
SMILES:	CCCCCCCCOC(C)(C)C
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	1156.00		NIST Webbook
tb	493.15	K	Joback Method
tc	663.06	K	Joback Method
tf	249.65	K	Joback Method
vc	0.715	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0010361	Paxs	330.82	Joback Method
dvisc	0.0005712	Paxs	371.40	Joback Method
dvisc	0.0003541	Paxs	411.98	Joback Method
dvisc	0.0002391	Paxs	452.57	Joback Method
dvisc	0.0001723	Paxs	493.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R559805&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

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

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