

Isobutyl tert-octyl ether

Inchi:	InChI=1S/C12H26O/c1-10(2)8-13-12(6,7)9-11(3,4)5/h10H,8-9H2,1-7H3
InchiKey:	UOTXTTHXUHAQMD-UHFFFAOYSA-N
Formula:	C12H26O
SMILES:	CC(C)COC(C)(C)CC(C)(C)C
Mol. weight [g/mol]:	186.33

Physical Properties

Property code	Value	Unit	Source
gf	-51.60	kJ/mol	Joback Method
hf	-446.01	kJ/mol	Joback Method
hfus	9.67	kJ/mol	Joback Method
hvap	41.74	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.874		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
rinpol	1077.00		NIST Webbook
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tb	489.48	K	Joback Method
tc	673.13	K	Joback Method
tf	237.07	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.51	J/molxK	489.48	Joback Method
cpg	528.07	J/molxK	642.52	Joback Method
cpg	512.36	J/molxK	611.92	Joback Method
cpg	495.78	J/molxK	581.31	Joback Method
cpg	478.31	J/molxK	550.70	Joback Method
cpg	459.90	J/molxK	520.09	Joback Method
cpg	542.95	J/molxK	673.13	Joback Method
dvisc	0.0001603	Paxs	489.48	Joback Method

dvisc	0.0002391	Paxs	447.41	Joback Method
dvisc	0.0003876	Paxs	405.34	Joback Method
dvisc	0.0007024	Paxs	363.27	Joback Method
dvisc	0.0014875	Paxs	321.21	Joback Method
dvisc	0.0039498	Paxs	279.14	Joback Method
dvisc	0.0148322	Paxs	237.07	Joback Method

Sources

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=R559761&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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