

Isobutyl octadecyl ether

Inchi:	InChI=1S/C22H46O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-21-22(2)3/h22
InchiKey:	WEDBUFYGSUBRTJ-UHFFFAOYSA-N
Formula:	C22H46O
SMILES:	CCCCCCCCCCCCCCCCCCOCC(C)C
Mol. weight [g/mol]:	326.60

Physical Properties

Property code	Value	Unit	Source
gf	26.92	kJ/mol	Joback Method
hf	-634.91	kJ/mol	Joback Method
hfus	50.40	kJ/mol	Joback Method
hvap	66.59	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	7.920		Crippen Method
mcvol	326.710	ml/mol	McGowan Method
pc	896.95	kPa	Joback Method
rinsol	2227.00		NIST Webbook
tb	724.74	K	Joback Method
tc	892.16	K	Joback Method
tf	344.93	K	Joback Method
vc	1.280	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.53	J/molxK	724.74	Joback Method
cpg	1019.37	J/molxK	752.64	Joback Method
cpg	1040.24	J/molxK	780.55	Joback Method
cpg	1060.15	J/molxK	808.45	Joback Method
cpg	1079.15	J/molxK	836.35	Joback Method
cpg	1097.25	J/molxK	864.26	Joback Method
cpg	1114.48	J/molxK	892.16	Joback Method
dvisc	0.0025238	Paxs	344.93	Joback Method
dvisc	0.0008050	Paxs	408.23	Joback Method

dvisc	0.0003489	Paxs	471.53	Joback Method
dvisc	0.0001844	Paxs	534.84	Joback Method
dvisc	0.0001115	Paxs	598.14	Joback Method
dvisc	0.0000742	Paxs	661.44	Joback Method
dvisc	0.0000531	Paxs	724.74	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=U406329&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

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