

Isobutyl hexadecyl ether

Inchi:	InChI=1S/C20H42O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-19-20(2)3/h20H,4-19H
InchiKey:	CZWWITYVYJRTOX-UHFFFAOYSA-N
Formula:	C20H42O
SMILES:	CCCCCCCCCCCCCCCCOCC(C)C
Mol. weight [g/mol]:	298.55

Physical Properties

Property code	Value	Unit	Source
gf	10.08	kJ/mol	Joback Method
hf	-593.63	kJ/mol	Joback Method
hfus	45.22	kJ/mol	Joback Method
hvap	62.14	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	7.140		Crippen Method
mcvol	298.530	ml/mol	McGowan Method
pc	1009.73	kPa	Joback Method
rinsol	2026.00		NIST Webbook
tb	678.98	K	Joback Method
tc	842.55	K	Joback Method
tf	322.39	K	Joback Method
vc	1.167	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.07	J/molxK	678.98	Joback Method
cpg	971.23	J/molxK	815.29	Joback Method
cpg	953.68	J/molxK	788.03	Joback Method
cpg	935.31	J/molxK	760.76	Joback Method
cpg	916.10	J/molxK	733.50	Joback Method
cpg	896.02	J/molxK	706.24	Joback Method
cpg	987.98	J/molxK	842.55	Joback Method
dvisc	0.0000693	Paxs	678.98	Joback Method
dvisc	0.0000967	Paxs	619.55	Joback Method

dvisc	0.0001447	Paxs	560.12	Joback Method
dvisc	0.0002382	Paxs	500.69	Joback Method
dvisc	0.0004487	Paxs	441.25	Joback Method
dvisc	0.0010291	Paxs	381.82	Joback Method
dvisc	0.0032060	Paxs	322.39	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=U406328&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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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