

Isopropyl octadecyl ether

Inchi:	InChI=1S/C21H44O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22-21(2)3/h21H,4
InchiKey:	DCZWEVHGJXFVJU-UHFFFAOYSA-N
Formula:	C21H44O
SMILES:	CCCCCCCCCCCCCCCCOC(C)C
Mol. weight [g/mol]:	312.57

Physical Properties

Property code	Value	Unit	Source
gf	18.50	kJ/mol	Joback Method
hf	-614.27	kJ/mol	Joback Method
hfus	47.81	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	7.673		Crippen Method
mcvol	312.620	ml/mol	McGowan Method
pc	950.84	kPa	Joback Method
rinsol	2125.00		NIST Webbook
tb	701.86	K	Joback Method
tc	867.07	K	Joback Method
tf	333.66	K	Joback Method
vc	1.224	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.80	J/molxK	701.86	Joback Method
cpg	1033.71	J/molxK	839.53	Joback Method
cpg	1015.89	J/molxK	812.00	Joback Method
cpg	997.21	J/molxK	784.46	Joback Method
cpg	977.65	J/molxK	756.93	Joback Method
cpg	957.19	J/molxK	729.39	Joback Method
cpg	1050.71	J/molxK	867.07	Joback Method
dvisc	0.0000608	Paxs	701.86	Joback Method
dvisc	0.0000849	Paxs	640.49	Joback Method

dvisc	0.0001272	Paxs	579.13	Joback Method
dvisc	0.0002100	Paxs	517.76	Joback Method
dvisc	0.0003964	Paxs	456.39	Joback Method
dvisc	0.0009120	Paxs	395.03	Joback Method
dvisc	0.0028507	Paxs	333.66	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406342&Units=SI

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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