

Dodecyl isobutyl ether

Inchi:	InChI=1S/C16H34O/c1-4-5-6-7-8-9-10-11-12-13-14-17-15-16(2)3/h16H,4-15H2,1-3H3
InchiKey:	BCNBKYACFICSFV-UHFFFAOYSA-N
Formula:	C16H34O
SMILES:	CCCCCCCCCCCCOCC(C)C
Mol. weight [g/mol]:	242.44

Physical Properties

Property code	Value	Unit	Source
gf	-23.60	kJ/mol	Joback Method
hf	-511.07	kJ/mol	Joback Method
hfus	34.86	kJ/mol	Joback Method
hvap	53.23	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	5.580		Crippen Method
mvol	242.170	ml/mol	McGowan Method
pc	1309.90	kPa	Joback Method
rinpol	1627.00		NIST Webbook
rinpol	1627.00		NIST Webbook
tb	587.46	K	Joback Method
tc	748.99	K	Joback Method
tf	277.31	K	Joback Method
vc	0.944	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.86	J/molxK	587.46	Joback Method
cpg	663.05	J/molxK	614.38	Joback Method
cpg	681.50	J/molxK	641.30	Joback Method
cpg	699.23	J/molxK	668.23	Joback Method
cpg	716.25	J/molxK	695.15	Joback Method
cpg	732.57	J/molxK	722.07	Joback Method
cpg	748.20	J/molxK	748.99	Joback Method
dvisc	0.0048619	Paxs	277.31	Joback Method

dvisc	0.0015862	Paxs	329.00	Joback Method
dvisc	0.0007015	Paxs	380.69	Joback Method
dvisc	0.0003771	Paxs	432.38	Joback Method
dvisc	0.0002314	Paxs	484.08	Joback Method
dvisc	0.0001560	Paxs	535.77	Joback Method
dvisc	0.0001128	Paxs	587.46	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=U406326&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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