

Isobutyl tetracosyl ether

Inchi: InChI=1S/C28H58O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28
InchiKey: BYHUQYLQWPAJPF-UHFFFAOYSA-N
Formula: C28H58O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCOCC(C)C
Mol. weight [g/mol]: 410.76

Physical Properties

Property code	Value	Unit	Source
gf	77.44	kJ/mol	Joback Method
hf	-758.75	kJ/mol	Joback Method
hfus	65.94	kJ/mol	Joback Method
hvap	79.94	kJ/mol	Joback Method
log10ws	-10.39		Crippen Method
logp	10.261		Crippen Method
mcvol	411.250	ml/mol	McGowan Method
pc	652.43	kPa	Joback Method
rinpol	2829.00		NIST Webbook
rinpol	2829.00		NIST Webbook
tb	862.02	K	Joback Method
tc	1058.17	K	Joback Method
tf	412.55	K	Joback Method
vc	1.615	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.93	J/molxK	862.02	Joback Method
cpg	1410.40	J/molxK	894.71	Joback Method
cpg	1434.43	J/molxK	927.40	Joback Method
cpg	1457.08	J/molxK	960.09	Joback Method
cpg	1478.38	J/molxK	992.79	Joback Method
cpg	1498.42	J/molxK	1025.48	Joback Method
cpg	1517.23	J/molxK	1058.17	Joback Method
dvisc	0.0011304	Paxs	412.55	Joback Method

dvisc	0.0003553	Paxs	487.46	Joback Method
dvisc	0.0001520	Paxs	562.37	Joback Method
dvisc	0.0000794	Paxs	637.28	Joback Method
dvisc	0.0000476	Paxs	712.20	Joback Method
dvisc	0.0000314	Paxs	787.11	Joback Method
dvisc	0.0000223	Paxs	862.02	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=U406332&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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