

Hexacosyl isobutyl ether

Inchi: InChI=1S/C30H62O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26
InchiKey: SRMLWYCPHSUWSY-UHFFFAOYSA-N
Formula: C30H62O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCOCC(C)C
Mol. weight [g/mol]: 438.81

Physical Properties

Property code	Value	Unit	Source
gf	94.28	kJ/mol	Joback Method
hf	-800.03	kJ/mol	Joback Method
hfus	71.12	kJ/mol	Joback Method
hvap	84.40	kJ/mol	Joback Method
log10ws	-11.23		Crippen Method
logp	11.041		Crippen Method
mcvol	439.430	ml/mol	McGowan Method
pc	592.86	kPa	Joback Method
rinpol	3027.00		NIST Webbook
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tb	907.78	K	Joback Method
tc	1121.15	K	Joback Method
tf	435.09	K	Joback Method
vc	1.728	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1518.98	J/molxK	907.78	Joback Method
cpg	1638.78	J/molxK	1085.59	Joback Method
cpg	1617.94	J/molxK	1050.03	Joback Method
cpg	1595.62	J/molxK	1014.47	Joback Method
cpg	1571.74	J/molxK	978.90	Joback Method
cpg	1546.22	J/molxK	943.34	Joback Method
cpg	1658.22	J/molxK	1121.15	Joback Method
dvisc	0.0000164	Paxs	907.78	Joback Method

dvisc	0.0000232	Paxs	829.00	Joback Method
dvisc	0.0000352	Paxs	750.22	Joback Method
dvisc	0.0000589	Paxs	671.43	Joback Method
dvisc	0.0001130	Paxs	592.65	Joback Method
dvisc	0.0002651	Paxs	513.87	Joback Method
dvisc	0.0008465	Paxs	435.09	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=U406333&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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