

Isopropyl hexacosyl ether

Inchi: InChI=1S/C29H60O/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: RKYZQQAFOCRQQJ-UHFFFAOYSA-N
Formula: C29H60O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(C)C
Mol. weight [g/mol]: 424.79

Physical Properties

Property code	Value	Unit	Source
gf	85.86	kJ/mol	Joback Method
hf	-779.39	kJ/mol	Joback Method
hfus	68.53	kJ/mol	Joback Method
hvap	82.17	kJ/mol	Joback Method
log10ws	-11.16		Crippen Method
logp	10.794		Crippen Method
mvol	425.340	ml/mol	McGowan Method
pc	621.58	kPa	Joback Method
rinpol	2921.00		NIST Webbook
rinpol	2921.00		NIST Webbook
tb	884.90	K	Joback Method
tc	1089.09	K	Joback Method
tf	423.82	K	Joback Method
vc	1.671	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1451.72	J/molxK	884.90	Joback Method
cpg	1478.03	J/molxK	918.93	Joback Method
cpg	1502.77	J/molxK	952.96	Joback Method
cpg	1526.01	J/molxK	986.99	Joback Method
cpg	1547.81	J/molxK	1021.02	Joback Method
cpg	1568.23	J/molxK	1055.06	Joback Method
cpg	1587.35	J/molxK	1089.09	Joback Method
dvisc	0.0009793	Paxs	423.82	Joback Method

dvisc	0.0003072	Paxs	500.67	Joback Method
dvisc	0.0001312	Paxs	577.51	Joback Method
dvisc	0.0000684	Paxs	654.36	Joback Method
dvisc	0.0000409	Paxs	731.21	Joback Method
dvisc	0.0000270	Paxs	808.05	Joback Method
dvisc	0.0000191	Paxs	884.90	Joback Method

Sources

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=U406346&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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