

Hexacosyl propyl ether

Inchi: InChI=1S/C29H60O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29
InchiKey: IIIXLTUYGXNPPS-UHFFFAOYSA-N
Formula: C29H60O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCOCCC
Mol. weight [g/mol]: 424.79

Physical Properties

Property code	Value	Unit	Source
gf	88.30	kJ/mol	Joback Method
hf	-774.11	kJ/mol	Joback Method
hfus	72.05	kJ/mol	Joback Method
hvap	82.56	kJ/mol	Joback Method
log10ws	-11.05		Crippen Method
logp	10.795		Crippen Method
mvol	425.340	ml/mol	McGowan Method
pc	619.10	kPa	Joback Method
rinpol	2982.00		NIST Webbook
rinpol	2982.00		NIST Webbook
tb	885.34	K	Joback Method
tc	1090.98	K	Joback Method
tf	438.82	K	Joback Method
vc	1.677	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1451.36	J/molxK	885.34	Joback Method
cpg	1477.87	J/molxK	919.61	Joback Method
cpg	1502.80	J/molxK	953.89	Joback Method
cpg	1526.22	J/molxK	988.16	Joback Method
cpg	1548.19	J/molxK	1022.44	Joback Method
cpg	1568.78	J/molxK	1056.71	Joback Method
cpg	1588.06	J/molxK	1090.98	Joback Method
dvisc	0.0007935	Paxs	438.82	Joback Method

dvisc	0.0002790	Paxs	513.24	Joback Method
dvisc	0.0001278	Paxs	587.66	Joback Method
dvisc	0.0000698	Paxs	662.08	Joback Method
dvisc	0.0000431	Paxs	736.50	Joback Method
dvisc	0.0000290	Paxs	810.92	Joback Method
dvisc	0.0000209	Paxs	885.34	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=U406284&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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