

1,3-Propanediol, ethyl tetracosyl ether

Inchi:	InChI=1S/C29H60O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey:	DPJMBSVCDUJOCA-UHFFFAOYSA-N
Formula:	C29H60O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCOCCOCC
Mol. weight [g/mol]:	440.79

Physical Properties

Property code	Value	Unit	Source
gf	-16.70	kJ/mol	Joback Method
hf	-906.33	kJ/mol	Joback Method
hfus	73.24	kJ/mol	Joback Method
hvap	84.97	kJ/mol	Joback Method
log10ws	-10.14		Crippen Method
logp	10.032		Crippen Method
mvol	431.210	ml/mol	McGowan Method
pc	613.90	kPa	Joback Method
rinpol	2970.00		NIST Webbook
rinpol	2970.00		NIST Webbook
tb	907.76	K	Joback Method
tc	1122.38	K	Joback Method
tf	461.05	K	Joback Method
vc	1.696	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1487.49	J/molxK	907.76	Joback Method
cpg	1603.25	J/molxK	1086.61	Joback Method
cpg	1583.42	J/molxK	1050.84	Joback Method
cpg	1561.99	J/molxK	1015.07	Joback Method
cpg	1538.90	J/molxK	979.30	Joback Method
cpg	1514.09	J/molxK	943.53	Joback Method
cpg	1621.55	J/molxK	1122.38	Joback Method
dvisc	0.0000155	Paxs	907.76	Joback Method

dvisc	0.0000214	Paxs	833.31	Joback Method
dvisc	0.0000314	Paxs	758.86	Joback Method
dvisc	0.0000504	Paxs	684.40	Joback Method
dvisc	0.0000905	Paxs	609.95	Joback Method
dvisc	0.0001913	Paxs	535.50	Joback Method
dvisc	0.0005153	Paxs	461.05	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=U406357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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