1,3-Propanediol, docosyl ethyl ether

Inchi: InChI=1S/C27H56O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-29
InchiKey: ITIOIGVBVLGYEE-UHFFFAOYSA-N
Formula: C27H56O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCOCCCOCC
Mol. weight [g/mol]: 412.73

Physical Properties

Property code	Value	Unit	Source
gf	-33.54	kJ/mol	Joback Method
hf	-865.05	kJ/mol	Joback Method
hfus	68.06	kJ/mol	Joback Method
hvap	80.52	kJ/mol	Joback Method
log10ws	-9.30		Crippen Method
logp	9.252		Crippen Method
mcvol	403.030	ml/mol	McGowan Method
pc	676.76	kPa	Joback Method
rinpol	2771.00		NIST Webbook
rinpol	2771.00		NIST Webbook
tb	862.00	K	Joback Method
tc	1058.81	K	Joback Method
tf	438.51	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1354.41	J/mol×K	862.00	Joback Method
cpg	1379.27	J/mol×K	894.80	Joback Method
cpg	1402.66	J/mol×K	927.60	Joback Method
cpg	1424.62	J/mol×K	960.40	Joback Method
cpg	1445.19	J/mol×K	993.21	Joback Method
cpg	1464.42	J/mol×K	1026.01	Joback Method
cpg	1482.34	J/mol×K	1058.81	Joback Method
dvisc	0.0006744	Pa×s	438.51	Joback Method

dvisc	0.0002533	Pa×s	509.09	Joback Method
dvisc	0.0001208	Pa×s	579.67	Joback Method
dvisc	0.0000676	Pa×s	650.25	Joback Method
dvisc	0.0000424	Pa×s	720.84	Joback Method
dvisc	0.0000289	Pa×s	791.42	Joback Method
dvisc	0.0000210	Pa×s	862.00	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U406356&Units=SI

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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