

Pentaethylene glycol, nonyl ether, acetate

Other names:	2-(2-(2-(2-(2-nonyloxy-ethoxy)-ethoxy)-ethoxy)-ethoxy)-ethanol, acetate
Inchi:	InChI=1S/C21H42O7/c1-3-4-5-6-7-8-9-10-23-11-12-24-13-14-25-15-16-26-17-18-27-19-20
InchiKey:	SJLONUQAWDWHBE-UHFFFAOYSA-N
Formula:	C21H42O7
SMILES:	CCCCCCCCCOCCOCCOCCOCCOCCOC(C)=O
Mol. weight [g/mol]:	406.55

Physical Properties

Property code	Value	Unit	Source
gf	-632.98	kJ/mol	Joback Method
hf	-1382.67	kJ/mol	Joback Method
hfus	58.87	kJ/mol	Joback Method
hvap	83.55	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	3.383		Crippen Method
mcvol	343.540	ml/mol	McGowan Method
pc	933.49	kPa	Joback Method
rinpol	2759.30		NIST Webbook
tb	868.27	K	Joback Method
tc	1063.80	K	Joback Method
tf	509.74	K	Joback Method
vc	1.325	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1134.12	J/molxK	868.27	Joback Method
cpg	1153.39	J/molxK	900.86	Joback Method
cpg	1171.17	J/molxK	933.45	Joback Method
cpg	1187.44	J/molxK	966.04	Joback Method
cpg	1202.17	J/molxK	998.62	Joback Method
cpg	1215.35	J/molxK	1031.21	Joback Method
cpg	1226.96	J/molxK	1063.80	Joback Method
dvisc	0.0002092	Paxs	509.74	Joback Method

dvisc	0.0001068	Paxs	569.50	Joback Method
dvisc	0.0000620	Paxs	629.25	Joback Method
dvisc	0.0000395	Paxs	689.00	Joback Method
dvisc	0.0000271	Paxs	748.76	Joback Method
dvisc	0.0000196	Paxs	808.51	Joback Method
dvisc	0.0000148	Paxs	868.27	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=R269062&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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