Heptaethylene glycol, pentyl ether, acetate

Other names: 2-(2-(2-(2-(2-(2-Pentoxy-ethoxy)-ethoxy)-ethoxy)-ethoxy)-ethoxy)-ethoxy)-ethyl acetate
Inchi: InChI=1S/C21H42O9/c1-3-4-5-6-23-7-8-24-9-10-25-11-12-26-13-14-27-15-16-28-17-18-2
InchiKey: ZCTDJKAUOOIYMM-UHFFFAOYSA-N
Formula: C21H42O9
SMILES: CCCCCOCCOCCOCCOCCOCCOCCOCCOC(C)=O
Mol. weight [g/mol]: 438.55

Physical Properties

Property code	Value	Unit	Source
gf	-842.98	kJ/mol	Joback Method
hf	-1647.11	kJ/mol	Joback Method
hfus	61.25	kJ/mol	Joback Method
hvap	88.37	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.856		Crippen Method
mcvol	355.280	ml/mol	McGowan Method
pc	914.39	kPa	Joback Method
rinpol	2918.30		NIST Webbook
rinpol	2918.30		NIST Webbook
tb	913.11	K	Joback Method
tc	1122.57	K	Joback Method
tf	554.20	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1197.49	J/mol×K	913.11	Joback Method
cpg	1215.94	J/mol×K	948.02	Joback Method
cpg	1232.43	J/mol×K	982.93	Joback Method
cpg	1246.90	J/mol×K	1017.84	Joback Method
cpg	1259.30	J/mol×K	1052.75	Joback Method
cpg	1269.58	J/mol×K	1087.66	Joback Method
cpg	1277.68	J/mol×K	1122.57	Joback Method

dvisc	0.0000969	Pa×s	554.20	Joback Method
dvisc	0.0000523	Pa×s	614.02	Joback Method
dvisc	0.0000315	Pa×s	673.84	Joback Method
dvisc	0.0000206	Pa×s	733.65	Joback Method
dvisc	0.0000143	Pa×s	793.47	Joback Method
dvisc	0.0000105	Pa×s	853.29	Joback Method
dvisc	0.0000080	Pa×s	913.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R188037&Units=SI
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

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