Pentaethylene glycol, monoallyl ether, acetate

Inchi: InChI=1S/C15H28O7/c1-3-4-17-5-6-18-7-8-19-9-10-20-11-12-21-13-14-22-15(2)16/h3H,1
InchiKey: ZEMNJRMFSLCADF-UHFFFAOYSA-N
Formula: C15H28O7
SMILES: C=CCOCCOCCOCCOCCOCCOC(C)=O
Mol. weight [g/mol]: 320.38

Physical Properties

Property code	Value	Unit	Source
gf	-595.66	kJ/mol	Joback Method
hf	-1133.40	kJ/mol	Joback Method
hfus	42.05	kJ/mol	Joback Method
hvap	69.52	kJ/mol	Joback Method
log10ws	-0.25		Crippen Method
logp	0.818		Crippen Method
mcvol	254.700	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	2076.00		NIST Webbook
rinpol	2077.00		NIST Webbook
rinpol	2075.00		NIST Webbook
tb	727.67	K	Joback Method
tc	901.36	K	Joback Method
tf	440.36	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.42	J/mol×K	727.67	Joback Method
cpg	763.48	J/mol×K	756.62	Joback Method
cpg	778.75	J/mol×K	785.57	Joback Method
cpg	793.19	J/mol×K	814.52	Joback Method
cpg	806.79	J/mol×K	843.47	Joback Method
cpg	819.52	J/mol×K	872.41	Joback Method
cpg	831.35	J/mol×K	901.36	Joback Method

dvisc	0.0004095	Pa×s	440.36	Joback Method
dvisc	0.0002276	Pa×s	488.25	Joback Method
dvisc	0.0001405	Pa×s	536.13	Joback Method
dvisc	0.0000939	Pa×s	584.01	Joback Method
dvisc	0.0000667	Pa×s	631.90	Joback Method
dvisc	0.0000497	Pa×s	679.78	Joback Method
dvisc	0.0000385	Pa×s	727.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R152231&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

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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