2-(2-(2-decyloxy-ethoxy)-ethoxy)-ethanol, acetate

Other names: Triethylene glycol, decyl ether, acetate
Inchi: InChI=1S/C18H36O5/c1-3-4-5-6-7-8-9-10-11-20-12-13-21-14-15-22-16-17-23-18(2)19/h3
InchiKey: FSXXCEPCQCGHQO-UHFFFAOYSA-N
Formula: C18H36O5
SMILES: CCCCCCCCCCOCCOCCOCCOC(C)=O
Mol. weight [g/mol]: 332.48

Physical Properties

Property code	Value	Unit	Source
gf	-448.24	kJ/mol	Joback Method
hf	-1056.31	kJ/mol	Joback Method
hfus	48.73	kJ/mol	Joback Method
hvap	72.05	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.740		Crippen Method
mcvol	289.530	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rinpol	2287.40		NIST Webbook
tb	754.79	K	Joback Method
tc	928.97	K	Joback Method
tf	431.47	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.98	J/mol×K	754.79	Joback Method
cpg	904.27	J/mol×K	783.82	Joback Method
cpg	921.64	J/mol×K	812.85	Joback Method
cpg	938.06	J/mol×K	841.88	Joback Method
cpg	953.56	J/mol×K	870.91	Joback Method
cpg	968.10	J/mol×K	899.94	Joback Method
cpg	981.71	J/mol×K	928.97	Joback Method
dvisc	0.0006347	Pa×s	431.47	Joback Method

dvisc	0.0003136	Pa×s	485.36	Joback Method
dvisc	0.0001784	Pa×s	539.24	Joback Method
dvisc	0.0001124	Pa×s	593.13	Joback Method
dvisc	0.0000765	Pa×s	647.02	Joback Method
dvisc	0.0000553	Pa×s	700.90	Joback Method
dvisc	0.0000418	Pa×s	754.79	Joback Method

Sources

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=R184293&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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