Triethylene glycol, amino, N-octyl

Inchi: InChI=1S/C14H31NO3/c1-2-3-4-5-6-7-8-15-9-11-17-13-14-18-12-10-16/h15-16H,2-14H2
InchiKey: XWQKDPZFMJPQGR-UHFFFAOYSA-N
Formula: C14H31NO3
SMILES: CCCCCCCCNCCOCCOCCO
Mol. weight [g/mol]: 261.40

Physical Properties

Property code	Value	Unit	Source
gf	-190.43	kJ/mol	Joback Method
hf	-695.49	kJ/mol	Joback Method
hfus	43.58	kJ/mol	Joback Method
hvap	74.69	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	1.962		Crippen Method
mcvol	235.710	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	1917.00		NIST Webbook
rinpol	1917.00		NIST Webbook
tb	706.91	K	Joback Method
tc	873.27	K	Joback Method
tf	405.48	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.80	J/mol×K	706.91	Joback Method
cpg	718.41	J/mol×K	734.64	Joback Method
cpg	733.34	J/mol×K	762.36	Joback Method
cpg	747.58	J/mol×K	790.09	Joback Method
cpg	761.15	J/mol×K	817.82	Joback Method
cpg	774.06	J/mol×K	845.54	Joback Method
cpg	786.31	J/mol×K	873.27	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=R120026&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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