Triethylene glycol, monothio, S-hexyl

Inchi: InChI=1S/C12H26O3S/c1-2-3-4-5-11-16-12-10-15-9-8-14-7-6-13/h13H,2-12H2,1H3
InchiKey: WRKMHGBLFGTHHZ-UHFFFAOYSA-N
Formula: C12H26O3S
SMILES: CCCCCCSCCOCCOCCO
Mol. weight [g/mol]: 250.40

Physical Properties

Property code	Value	Unit	Source
gf	-263.54	kJ/mol	Joback Method
hf	-665.81	kJ/mol	Joback Method
hfus	37.43	kJ/mol	Joback Method
hvap	70.62	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	2.325		Crippen Method
mcvol	213.900	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1844.00		NIST Webbook
rinpol	1844.00		NIST Webbook
tb	679.76	K	Joback Method
tc	852.95	K	Joback Method
tf	364.68	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.55	J/mol×K	679.76	Joback Method
cpg	611.00	J/mol×K	708.62	Joback Method
cpg	624.80	J/mol×K	737.49	Joback Method
cpg	637.95	J/mol×K	766.35	Joback Method
cpg	650.45	J/mol×K	795.22	Joback Method
cpg	662.31	J/mol×K	824.08	Joback Method
cpg	673.53	J/mol×K	852.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R120071&Units=SI

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