Diethylene glycol, thio, S-octyl

Inchi: InChI=1S/C12H26O2S/c1-2-3-4-5-6-7-11-15-12-10-14-9-8-13/h13H,2-12H2,1H3
InchiKey: OPFRXVSGBZCPFM-UHFFFAOYSA-N
Formula: C12H26O2S
SMILES: CCCCCCCCSCCOCCO
Mol. weight [g/mol]: 234.40

Physical Properties

Property code	Value	Unit	Source
gf	-158.54	kJ/mol	Joback Method
hf	-533.59	kJ/mol	Joback Method
hfus	36.24	kJ/mol	Joback Method
hvap	68.21	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	3.089		Crippen Method
mcvol	208.030	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
tb	657.34	K	Joback Method
tc	830.04	K	Joback Method
tf	342.45	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.53	J/mol×K	657.34	Joback Method
cpg	583.10	J/mol×K	686.12	Joback Method
cpg	597.03	J/mol×K	714.91	Joback Method
cpg	610.33	J/mol×K	743.69	Joback Method
cpg	623.00	J/mol×K	772.47	Joback Method
cpg	635.05	J/mol×K	801.26	Joback Method
cpg	646.50	J/mol×K	830.04	Joback Method

Sources

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=R120006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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