Diethylene glycol, monothio, S-hexyl

Inchi: InChI=1S/C10H22O2S/c1-2-3-4-5-9-13-10-8-12-7-6-11/h11H,2-10H2,1H3
InchiKey: RZRAIUMCYHFWCL-UHFFFAOYSA-N
Formula: C10H22O2S
SMILES: CCCCCCSCCOCCO
Mol. weight [g/mol]: 206.34

Physical Properties

Property code	Value	Unit	Source
gf	-175.38	kJ/mol	Joback Method
hf	-492.31	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	63.76	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.309		Crippen Method
mcvol	179.850	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1578.00		NIST Webbook
rinpol	1578.00		NIST Webbook
tb	611.58	K	Joback Method
tc	785.50	K	Joback Method
tf	319.91	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.90	J/mol×K	611.58	Joback Method
cpg	478.24	J/mol×K	640.57	Joback Method
cpg	491.03	J/mol×K	669.55	Joback Method
cpg	503.26	J/mol×K	698.54	Joback Method
cpg	514.95	J/mol×K	727.53	Joback Method
cpg	526.09	J/mol×K	756.51	Joback Method
cpg	536.70	J/mol×K	785.50	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=R119992&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