2-[2-(heptyloxy)ethoxy]ethanol

Other names: diethylene glycol heptyl ether
diethylene glycol mono(n-heptyl) ether
diethylene glycol monoheptyl ether
ethanol, 2-[2-(heptyloxy)ethoxy]-
Inchi: InChI=1S/C11H24O3/c1-2-3-4-5-6-8-13-10-11-14-9-7-12/h12H,2-11H2,1H3
InchiKey: OVPQPMTZOLCPHB-UHFFFAOYSA-N
Formula: C11H24O3
SMILES: CCCCCCCOCCOCCO
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
af	0.8772		Cheméo Relay (1.0)
gf	-305.08	kJ/mol	Joback Method
hf	-684.25	kJ/mol	Cheméo Relay (1.0)
hfus	30.71	kJ/mol	Joback Method
hvap	81.01	kJ/mol	Cheméo Relay (1.0)
ie	9.77	eV	Cheméo Relay (1.0)
log10ws	-1.97		Cheméo Relay (1.0)
logp	1.982		Crippen Method
mcvol	183.460	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
tb	554.28	K	Cheméo Relay (1.0)
tc	726.20	K	Cheméo Relay (1.0)
tf	255.32	K	Cheméo Relay (1.0)
vc	0.704	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.23	J/mol×K	588.10	Joback Method
cpg	558.19	J/mol×K	746.96	Joback Method
cpg	546.89	J/mol×K	720.48	Joback Method
cpg	535.12	J/mol×K	694.01	Joback Method

cpg	522.87	J/mol×K	667.53	Joback Method
cpg	510.14	J/mol×K	641.05	Joback Method
cpg	496.93	J/mol×K	614.58	Joback Method
dvisc	0.0002968	Pa×s	453.55	Joback Method
dvisc	0.0000559	Pa×s	588.10	Joback Method
dvisc	0.0000889	Pa×s	543.25	Joback Method
dvisc	0.0001539	Pa×s	498.40	Joback Method
dvisc	0.0064440	Pa×s	319.01	Joback Method
dvisc	0.0006610	Pa×s	408.71	Joback Method
dvisc	0.0017937	Pa×s	363.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Mutual Solubility and Lower Critical Solution Temperature for Water + Glycol Ether Systems:	https://www.doi.org/10.1021/je049635u
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume