

Ethanol, 2-(heptyloxy)-

Other names:	2-(heptyloxy)ethanol ethylene glycol mono-n-heptyl ether ethylene glycol monoheptyl ether heptyl cellosolve
Inchi:	InChI=1S/C9H20O2/c1-2-3-4-5-6-8-11-9-7-10/h10H,2-9H2,1H3
InchiKey:	QJTOHHRPYAVWOO-UHFFFAOYSA-N
Formula:	C9H20O2
SMILES:	CCCCCCCOCO
Mol. weight [g/mol]:	160.25
CAS:	7409-44-1

Physical Properties

Property code	Value	Unit	Source
gf	-216.92	kJ/mol	Joback Method
hf	-513.54	kJ/mol	Joback Method
hfus	24.34	kJ/mol	Joback Method
hvap	54.72	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.966		Crippen Method
mcvol	149.410	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
tb	519.92	K	Joback Method
tc	679.11	K	Joback Method
tf	274.24	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.86	J/molxK	519.92	Joback Method
cpg	372.13	J/molxK	546.45	Joback Method
cpg	383.97	J/molxK	572.98	Joback Method
cpg	395.39	J/molxK	599.51	Joback Method
cpg	406.39	J/molxK	626.04	Joback Method

cpg	416.99	J/molxK	652.58	Joback Method
cpg	427.19	J/molxK	679.11	Joback Method
dvisc	0.0194190	Paxs	274.24	Joback Method
dvisc	0.0046894	Paxs	315.19	Joback Method
dvisc	0.0015701	Paxs	356.13	Joback Method
dvisc	0.0006587	Paxs	397.08	Joback Method
dvisc	0.0003251	Paxs	438.03	Joback Method
dvisc	0.0001810	Paxs	478.97	Joback Method
dvisc	0.0001106	Paxs	519.92	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Mutual Solubility and Lower Critical Solution Temperature for Water + Organic Systems:	https://www.doi.org/10.1021/je049635u
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=C7409441&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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