

Ethanol, 2-(2-hydroxyethoxy)-, 1-nitrate

Other names:	Diethylene glycol, mononitrate Ethanol, 2,2'-oxybis-, mononitrate
Inchi:	InChI=1S/C4H9NO5/c6-1-2-9-3-4-10-5(7)8/h6H,1-4H2
InchiKey:	QRCYUCUXPSBJNO-UHFFFAOYSA-N
Formula:	C4H9NO5
SMILES:	O=[N+](O-)OCCOCCO
Mol. weight [g/mol]:	151.12
CAS:	20633-16-3

Physical Properties

Property code	Value	Unit	Source
gf	-328.47	kJ/mol	Joback Method
hf	-553.32	kJ/mol	Joback Method
hfus	23.94	kJ/mol	Joback Method
hvap	62.59	kJ/mol	Joback Method
log10ws	-9.51e-03		Crippen Method
logp	-0.796		Crippen Method
mvol	102.250	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
tb	579.78	K	Joback Method
tc	771.47	K	Joback Method
tf	383.73	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.00	J/molxK	579.78	Joback Method
cpg	259.93	J/molxK	611.73	Joback Method
cpg	267.54	J/molxK	643.68	Joback Method
cpg	274.80	J/molxK	675.63	Joback Method
cpg	281.73	J/molxK	707.57	Joback Method
cpg	288.30	J/molxK	739.52	Joback Method
cpg	294.50	J/molxK	771.47	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=C20633163&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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