

2-ETHYL-2-NITROPROPANE-1,3-DIOL

Other names:	1,3-Propanediol, 2-ethyl-2-nitro- 2-Ethyl-2-nitropropanediol 2-Ethyl-2-nitro-1,3-propanediol NEPD 2-ethyl-2-nitropropane-1,3-diol
Inchi:	InChI=1S/C5H11NO4/c1-2-5(3-7,4-8)6(9)10/h7-8H,2-4H2,1H3
InchiKey:	YADISKICBOYXFS-UHFFFAOYSA-N
Formula:	C5H11NO4
SMILES:	CCC(CO)(CO)[N+](=O)[O-]
Mol. weight [g/mol]:	149.15

Physical Properties

Property code	Value	Unit	Source
chs	-2938.00	kJ/mol	NIST Webbook
chs	-2931.90 ± 1.30	kJ/mol	NIST Webbook
hfs	-601.20	kJ/mol	NIST Webbook
hfs	-607.70 ± 1.40	kJ/mol	NIST Webbook
hfus	20.83	kJ/mol	Joback Method
logp	-0.604		Crippen Method
mcvol	110.470	ml/mol	McGowan Method
tf	370.82	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.50	J/mol×K	646.77	Joback Method
cpg	306.20	J/mol×K	678.72	Joback Method
cpg	313.42	J/mol×K	710.66	Joback Method
cpg	320.20	J/mol×K	742.61	Joback Method
cpg	326.56	J/mol×K	774.55	Joback Method
cpg	332.54	J/mol×K	806.50	Joback Method
cpg	338.16	J/mol×K	838.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C597091&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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