1,5-Pentanediol, dinitrate

Other names: 5-nitrooxypentyl nitrate
Pentamethylene dinitrate
Pentamethylene nitrate
Inchi: InChI=1S/C5H10N2O6/c8-6(9)12-4-2-1-3-5-13-7(10)11/h1-5H2
InchiKey: MIYIEPHJPVBSEV-UHFFFAOYSA-N
Formula: C5H10N2O6
SMILES: O=[N+]([O-])OCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]: 194.14
CAS: 3457-92-9

Physical Properties

Property code	Value	Unit	Source
chl	-3035.00	kJ/mol	NIST Webbook
gf	-147.68	kJ/mol	Joback Method
hf	-432.49	kJ/mol	Joback Method
hfus	33.80	kJ/mol	Joback Method
hvap	64.73	kJ/mol	Joback Method
log10ws	-2.19		Aqueous Solubility Prediction Method
logp	0.573		Crippen Method
mcvol	127.890	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
rinpol	1329.00		NIST Webbook
tb	662.32	K	Joback Method
tc	888.40	K	Joback Method
tf	256.60 ± 0.10	K	NIST Webbook
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.76	J/mol×K	662.32	Joback Method
cpg	349.00	J/mol×K	700.00	Joback Method
cpg	358.58	J/mol×K	737.68	Joback Method

cpg	367.51	J/mol×K	775.36	Joback Method
cpg	375.78	J/mol×K	813.04	Joback Method
cpg	383.37	J/mol×K	850.72	Joback Method
cpg	390.29	J/mol×K	888.40	Joback Method
hvapt	78.90 ± 5.90	kJ/mol	303.00	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3457929&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chl: Standard liquid enthalpy of combustion
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
hvapt: Enthalpy of vaporization at a given temperature
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