2,4-Pentanediol dinitrate

Other names: 4-nitrooxypentan-2-yl nitrate
Inchi: InChI=1S/C5H10N2O6/c1-4(12-6(8)9)3-5(2)13-7(10)11/h4-5H,3H2,1-2H3
InchiKey: XVWLQUXGMQFTPO-UHFFFAOYSA-N
Formula: C5H10N2O6
SMILES: CC(CC(C)O[N+](=O)[O-])O[N+](=O)[O-]
Mol. weight [g/mol]: 194.14
CAS: 101421-04-9

Physical Properties

Property code	Value	Unit	Source
chl	-3012.00	kJ/mol	NIST Webbook
hf	-321.80	kJ/mol	Cheméo Relay (1.0)
hfl	-386.00	kJ/mol	NIST Webbook
hfus	26.76	kJ/mol	Joback Method
hvap	73.83	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.22		Aqueous Solubility Prediction Method
logp	0.570		Crippen Method
mcvol	127.890	ml/mol	McGowan Method
tb	456.90	K	Cheméo Relay (1.0)
tf	265.99	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.89	J/mol×K	661.44	Joback Method
cpg	350.62	J/mol×K	700.68	Joback Method
cpg	360.62	J/mol×K	739.91	Joback Method
cpg	369.87	J/mol×K	779.15	Joback Method
cpg	378.39	J/mol×K	818.39	Joback Method
cpg	386.14	J/mol×K	857.62	Joback Method
cpg	393.14	J/mol×K	896.86	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101421049&Units=SI&Mask=3FFF

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point