

1,4-pentanediol, dinitrate

Other names:	2,4-Pentanediol dinitrate 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:	25385-63-1

Physical Properties

Property code	Value	Unit	Source
gf	-152.56	kJ/mol	Joback Method
hf	-443.05	kJ/mol	Joback Method
hfus	26.76	kJ/mol	Joback Method
hvap	63.95	kJ/mol	Joback Method
log10ws	-2.22		Aqueous Solubility Prediction Method
logp	0.570		Crippen Method
mcvol	127.890	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
tb	661.44	K	Joback Method
tc	896.86	K	Joback Method
tf	254.70 ± 0.10	K	NIST Webbook
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

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

cpg	393.14	J/mol×K	896.86	Joback Method
hvapt	60.60 ± 5.90	kJ/mol	303.00	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C25385631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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