

Erythrityl tetranitrate

Inchi:	InChI=1S/C4H6N4O12/c9-5(10)17-1-3(19-7(13)14)4(20-8(15)16)2-18-6(11)12/h3-4H,1-2
InchiKey:	SNFOERUNNSHUGP-UHFFFAOYSA-N
Formula:	C4H6N4O12
SMILES:	O=[N+]([O-])OCC(O[N+](=O)[O-])C(CO[N+](=O)[O-])O[N+](=O)[O-]
Mol. weight [g/mol]:	302.11
CAS:	142435-64-1

Physical Properties

Property code	Value	Unit	Source
gf	-299.88	kJ/mol	Joback Method
hf	-708.37	kJ/mol	Joback Method
hfus	49.27	kJ/mol	Joback Method
hvap	99.73	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	-1.443		Crippen Method
mcvol	160.380	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
tb	987.08	K	Joback Method
tc	1252.73	K	Joback Method
tf	768.20	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.51	J/molxK	987.08	Joback Method
cpg	488.03	J/molxK	1031.36	Joback Method
cpg	490.02	J/molxK	1075.63	Joback Method
cpg	490.41	J/molxK	1119.91	Joback Method
cpg	489.15	J/molxK	1164.18	Joback Method
cpg	486.18	J/molxK	1208.46	Joback Method
cpg	481.45	J/molxK	1252.73	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=C142435641&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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