

2,4,6-Trinitrophenoxyethyl nitrate

Inchi:	InChI=1S/C8H6N4O10/c13-7(3-22-12(20)21)8-5(10(16)17)1-4(9(14)15)2-6(8)11(18)19/h
InchiKey:	FZGJOYSOYXPXNM-UHFFFAOYSA-N
Formula:	C8H6N4O10
SMILES:	O=[N+]([O-])OCC(O)c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	318.15
CAS:	62030-33-5

Physical Properties

Property code	Value	Unit	Source
chs	-3718.10	kJ/mol	NIST Webbook
chs	-3718.00 ± 3.70	kJ/mol	NIST Webbook
gf	-2.06	kJ/mol	Joback Method
hf	-339.10	kJ/mol	Joback Method
hfs	-287.70	kJ/mol	NIST Webbook
hfs	-287.50 ± 3.70	kJ/mol	NIST Webbook
hfus	56.55	kJ/mol	Joback Method
hvap	122.73	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	0.653		Crippen Method
mcvol	181.240	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
tb	1145.58	K	Joback Method
tc	1422.79	K	Joback Method
tf	886.39	K	Joback Method
vc	0.735	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.51	J/mol×K	1145.58	Joback Method
cpg	542.58	J/mol×K	1191.78	Joback Method
cpg	543.65	J/mol×K	1237.98	Joback Method
cpg	543.77	J/mol×K	1284.19	Joback Method
cpg	542.98	J/mol×K	1330.39	Joback Method

cpg	541.31	J/mol×K	1376.59	Joback Method
cpg	538.82	J/mol×K	1422.79	Joback Method

Sources

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=C62030335&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid 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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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