1,3-Propanediol, 2-methyl-2-n-propyl-, dinitrate

Other names: 2-methyl-2-propylpropane-1,3-diyl dinitrate
Inchi: InChI=1S/C7H14N2O6/c1-3-4-7(2,5-14-8(10)11)6-15-9(12)13/h3-6H2,1-2H3
InchiKey: BLJBDLGFKNXUCB-UHFFFAOYSA-N
Formula: C7H14N2O6
SMILES: CCCC(C)(CO[N+](=O)[O-])CO[N+](=O)[O-]
Mol. weight [g/mol]: 222.20
CAS: 10605-24-0

Physical Properties

Property code	Value	Unit	Source
gf	-128.00	kJ/mol	Joback Method
hf	-482.52	kJ/mol	Joback Method
hfus	31.57	kJ/mol	Joback Method
hvap	67.88	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	1.209		Crippen Method
mcvol	156.070	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
tb	704.85	K	Joback Method
tc	935.06	K	Joback Method
tf	502.75	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.70	J/mol×K	704.85	Joback Method
cpg	452.67	J/mol×K	743.22	Joback Method
cpg	463.77	J/mol×K	781.59	Joback Method
cpg	474.01	J/mol×K	819.95	Joback Method
cpg	483.42	J/mol×K	858.32	Joback Method
cpg	492.02	J/mol×K	896.69	Joback Method
cpg	499.85	J/mol×K	935.06	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C10605240&Units=SI

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
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