

Glycolic acid, nitrate, isopropyl ester

Inchi:	InChI=1S/C5H9NO5/c1-4(2)11-5(7)3-10-6(8)9/h4H,3H2,1-2H3
InchiKey:	VCIBYKQFLWINFO-UHFFFAOYSA-N
Formula:	C5H9NO5
SMILES:	CC(C)OC(=O)CO[N+](=O)[O-]
Mol. weight [g/mol]:	163.13

Physical Properties

Property code	Value	Unit	Source
gf	-314.59	kJ/mol	Joback Method
hf	-539.59	kJ/mol	Joback Method
hfus	20.52	kJ/mol	Joback Method
hvap	54.49	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	0.146		Crippen Method
mcvol	112.040	ml/mol	McGowan Method
pc	3677.55	kPa	Joback Method
rinpola	1010.00		NIST Webbook
tb	563.91	K	Joback Method
tc	778.27	K	Joback Method
tf	369.11	K	Joback Method
vc	0.433	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.34	J/mol×K	563.91	Joback Method
cpg	275.13	J/mol×K	599.64	Joback Method
cpg	284.47	J/mol×K	635.36	Joback Method
cpg	293.32	J/mol×K	671.09	Joback Method
cpg	301.69	J/mol×K	706.81	Joback Method
cpg	309.56	J/mol×K	742.54	Joback Method
cpg	316.90	J/mol×K	778.27	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R633057&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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