

cyclohexylnitrate

Inchi:	InChI=1S/C6H11NO3/c8-7(9)10-6-4-2-1-3-5-6/h6H,1-5H2
InchiKey:	HLYOOCIMLHNMOG-UHFFFAOYSA-N
Formula:	C6H11NO3
SMILES:	O=[N+](O-)OC1CCCCC1
Mol. weight [g/mol]:	145.16
CAS:	2108-66-9

Physical Properties

Property code	Value	Unit	Source
gf	-45.36	kJ/mol	Joback Method
hf	-255.83	kJ/mol	Joback Method
hfus	15.68	kJ/mol	Joback Method
hvap	48.38	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	1.527		Crippen Method
mcvol	107.830	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	530.49	K	Joback Method
tc	771.79	K	Joback Method
tf	330.60	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.59	J/molxK	530.49	Joback Method
cpg	272.76	J/molxK	570.71	Joback Method
cpg	286.98	J/molxK	610.92	Joback Method
cpg	300.28	J/molxK	651.14	Joback Method
cpg	312.67	J/molxK	691.36	Joback Method
cpg	324.15	J/molxK	731.57	Joback Method
cpg	334.74	J/molxK	771.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2108669&Units=SI
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

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
mccvol:	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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