L-Homoserine lactone, N-heptafluorobutyryl-

Inchi: InChI=1S/C8H6F7NO3/c9-6(10,7(11,12)8(13,14)15)5(18)16-3-1-2-19-4(3)17/h3H,1-2H2,
InchiKey: YITYWEDIUXKOKO-UHFFFAOYSA-N
Formula: C8H6F7NO3
SMILES: O=C1OCCC1NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 297.13

Physical Properties

Property code	Value	Unit	Source
gf	-1550.36	kJ/mol	Joback Method
hf	-1875.80	kJ/mol	Joback Method
hfus	23.92	kJ/mol	Joback Method
hvap	45.99	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.251		Crippen Method
mcvol	144.100	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	1231.00		NIST Webbook
tb	581.73	K	Joback Method
tc	769.59	K	Joback Method
tf	399.59	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.55	J/mol×K	581.73	Joback Method
cpg	425.59	J/mol×K	613.04	Joback Method
cpg	436.72	J/mol×K	644.35	Joback Method
cpg	446.98	J/mol×K	675.66	Joback Method
cpg	456.42	J/mol×K	706.97	Joback Method
cpg	465.09	J/mol×K	738.28	Joback Method
cpg	473.04	J/mol×K	769.59	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=U374763&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume