Cyclamat (cyclohexaneaminosulfonic acid) methyl ester

Inchi: InChI=1S/C7H15NO3S/c1-11-12(9,10)8-7-5-3-2-4-6-7/h7-8H,2-6H2,1H3
InchiKey: MCKYCQMLMPAYIV-UHFFFAOYSA-N
Formula: C7H15NO3S
SMILES: COS(=O)(=O)NC1CCCCC1
Mol. weight [g/mol]: 193.26

Physical Properties

Property code	Value	Unit	Source
gf	-451.64	kJ/mol	Joback Method
hf	-665.59	kJ/mol	Joback Method
hfus	23.39	kJ/mol	Joback Method
hvap	59.09	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	0.800		Crippen Method
mcvol	142.570	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
rinpol	1528.00		NIST Webbook
tb	499.48	K	Joback Method
tc	698.78	K	Joback Method
tf	289.48	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.22	J/mol×K	499.48	Joback Method
cpg	342.72	J/mol×K	532.70	Joback Method
cpg	358.45	J/mol×K	565.91	Joback Method
cpg	373.40	J/mol×K	599.13	Joback Method
cpg	387.57	J/mol×K	632.35	Joback Method
cpg	400.94	J/mol×K	665.56	Joback Method
cpg	413.51	J/mol×K	698.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R524864&Units=SI
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

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