1-methylbicyclo[3.3.0]-2,8-dioxa-4-thiaoctane

Inchi: InChI=1S/C6H10O2S/c1-6-5(2-3-7-6)9-4-8-6/h5H,2-4H2,1H3
InchiKey: DTZCQCZGDSIIQI-UHFFFAOYSA-N
Formula: C6H10O2S
SMILES: CC12OCCC1SCO2
Mol. weight [g/mol]: 146.21

Physical Properties

Property code	Value	Unit	Source
gf	-40.93	kJ/mol	Joback Method
hf	-237.39	kJ/mol	Joback Method
hfus	16.68	kJ/mol	Joback Method
hvap	42.80	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	1.212		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	4672.09	kPa	Joback Method
ripol	1642.00		NIST Webbook
tb	460.67	K	Joback Method
tc	701.81	K	Joback Method
tf	346.71	K	Joback Method
vc	0.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.72	J/mol×K	460.67	Joback Method
cpg	239.47	J/mol×K	500.86	Joback Method
cpg	252.80	J/mol×K	541.05	Joback Method
cpg	264.90	J/mol×K	581.24	Joback Method
cpg	275.96	J/mol×K	621.43	Joback Method
cpg	286.17	J/mol×K	661.62	Joback Method
cpg	295.72	J/mol×K	701.81	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=R169165&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume