

1,6-Dioxaspiro[4.4]nonane-2,7-dione

Inchi:	InChI=1S/C7H8O4/c8-5-1-3-7(10-5)4-2-6(9)11-7/h1-4H2
InchiKey:	VTQYOGUFKHWOO-UHFFFAOYSA-N
Formula:	C7H8O4
SMILES:	O=C1CCC2(CCC(=O)O2)O1
Mol. weight [g/mol]:	156.14
CAS:	3505-67-7

Physical Properties

Property code	Value	Unit	Source
gf	-321.94	kJ/mol	Joback Method
hf	-564.51	kJ/mol	Joback Method
hfus	11.46	kJ/mol	Joback Method
hvap	48.19	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	0.357		Crippen Method
mcvol	102.650	ml/mol	McGowan Method
pc	4924.59	kPa	Joback Method
tb	580.30	K	Joback Method
tc	846.12	K	Joback Method
tf	411.69	K	Joback Method
vc	0.372	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.32	J/molxK	580.30	Joback Method
cpg	284.72	J/molxK	624.60	Joback Method
cpg	298.19	J/molxK	668.91	Joback Method
cpg	310.86	J/molxK	713.21	Joback Method
cpg	322.89	J/molxK	757.51	Joback Method
cpg	334.40	J/molxK	801.82	Joback Method
cpg	345.54	J/molxK	846.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3505677&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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