2,2,7,7-tetramethyl-1,6-dioxaspiro[4.4]nona-3,8-di

Inchi: InChI=1S/C11H16O2/c1-9(2)5-7-11(12-9)8-6-10(3,4)13-11/h5-8H,1-4H3
InchiKey: XBYJEPZKXGPIKK-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: CC1(C)C=CC2(C=CC(C)(C)O2)O1
Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
gf	-9.56	kJ/mol	Joback Method
hf	-266.31	kJ/mol	Joback Method
hfus	14.79	kJ/mol	Joback Method
hvap	46.26	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.413		Crippen Method
mcvol	147.270	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
ripol	1288.00		NIST Webbook
tb	525.64	K	Joback Method
tc	765.78	K	Joback Method
tf	361.17	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.59	J/mol×K	525.64	Joback Method
cpg	384.29	J/mol×K	565.66	Joback Method
cpg	400.31	J/mol×K	605.69	Joback Method
cpg	415.07	J/mol×K	645.71	Joback Method
cpg	428.99	J/mol×K	685.73	Joback Method
cpg	442.49	J/mol×K	725.75	Joback Method
cpg	455.98	J/mol×K	765.78	Joback Method

Sources

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=R307530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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