1,3,3,4,6,6-Hexamethyl-2,5,7-trioxabicyclo[2.2.1]he

Inchi: InChI=1S/C10H18O3/c1-7(2)9(5)12-8(3,4)10(6,11-7)13-9/h1-6H3
InchiKey: VKNKFXJFQVTQKD-UHFFFAOYSA-N
Formula: C10H18O3
SMILES: CC1(C)OC2(C)OC1(C)OC2(C)C
Mol. weight [g/mol]: 186.25
CAS: 7045-89-8

Physical Properties

Property code	Value	Unit	Source
gf	-153.02	kJ/mol	Joback Method
hf	-486.01	kJ/mol	Joback Method
hfus	16.71	kJ/mol	Joback Method
hvap	46.16	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.053		Crippen Method
mcvol	147.650	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	518.42	K	Joback Method
tc	747.96	K	Joback Method
tf	401.65	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.08	J/mol×K	518.42	Joback Method
cpg	404.08	J/mol×K	556.68	Joback Method
cpg	419.40	J/mol×K	594.93	Joback Method
cpg	433.48	J/mol×K	633.19	Joback Method
cpg	446.81	J/mol×K	671.45	Joback Method
cpg	459.85	J/mol×K	709.70	Joback Method
cpg	473.05	J/mol×K	747.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7045898&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