2-t-Butyl-5-propyl-[1,3]dioxolan-4-one

Other names: 2-tert-Butyl-5-propyl-(1,3)dioxolan-4-one
Inchi: InChI=1S/C10H18O3/c1-5-6-7-8(11)13-9(12-7)10(2,3)4/h7,9H,5-6H2,1-4H3
InchiKey: ILGODMRZDJWLOV-UHFFFAOYSA-N
Formula: C10H18O3
SMILES: CCCC1OC(C(C)(C)C)OC1=O
Mol. weight [g/mol]: 186.25
CAS: 157733-17-0

Physical Properties

Property code	Value	Unit	Source
gf	-229.83	kJ/mol	Joback Method
hf	-620.04	kJ/mol	Joback Method
hfus	24.72	kJ/mol	Joback Method
hvap	49.77	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.101		Crippen Method
mcvol	154.210	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
rinpol	1432.00		NIST Webbook
tb	557.30	K	Joback Method
tc	772.74	K	Joback Method
tf	332.90	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.67	J/mol×K	557.30	Joback Method
cpg	424.78	J/mol×K	593.21	Joback Method
cpg	441.91	J/mol×K	629.11	Joback Method
cpg	458.05	J/mol×K	665.02	Joback Method
cpg	473.25	J/mol×K	700.93	Joback Method
cpg	487.50	J/mol×K	736.83	Joback Method
cpg	500.82	J/mol×K	772.74	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=C157733170&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume