2-Methyl-5-(propan-2-ylidene)cyclohexane-1,4-dio

Inchi: InChI=1S/C10H18O2/c1-6(2)8-5-9(11)7(3)4-10(8)12/h7,9-12H,4-5H2,1-3H3
InchiKey: UGOBXYSHUVWTRV-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC(C)=C1CC(O)C(C)CC1O
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-194.38	kJ/mol	Joback Method
hf	-474.31	kJ/mol	Joback Method
hfus	22.82	kJ/mol	Joback Method
hvap	71.89	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.475		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	1321.80		NIST Webbook
tb	629.29	K	Joback Method
tc	814.13	K	Joback Method
tf	319.40	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.80	J/mol×K	629.29	Joback Method
cpg	427.48	J/mol×K	660.10	Joback Method
cpg	440.49	J/mol×K	690.90	Joback Method
cpg	452.83	J/mol×K	721.71	Joback Method
cpg	464.53	J/mol×K	752.52	Joback Method
cpg	475.59	J/mol×K	783.33	Joback Method
cpg	486.03	J/mol×K	814.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413841&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume