1,2,3,6-tetrahydromethyl-3,6-methanophthalic anhydride

Inchi: InChI=1S/C10H12O3/c1-4-5-2-3-6(4)8-7(5)9(11)13-10(8)12/h4-8H,2-3H2,1H3
InchiKey: OCCLSAYXEPHUMI-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: CC1C2CCC1C1C(=O)OC(=O)C21
Mol. weight [g/mol]: 180.20
CAS: 25134-21-8

Physical Properties

Property code	Value	Unit	Source
gf	-143.25	kJ/mol	Joback Method
hf	-485.57	kJ/mol	Joback Method
hfus	23.10	kJ/mol	Joback Method
hvap	50.15	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	0.978		Crippen Method
mcvol	128.190	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
tb	605.94	K	Joback Method
tc	848.78	K	Joback Method
tf	407.29	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.86	J/mol×K	605.94	Joback Method
cpg	394.10	J/mol×K	646.41	Joback Method
cpg	411.17	J/mol×K	686.89	Joback Method
cpg	427.10	J/mol×K	727.36	Joback Method
cpg	441.93	J/mol×K	767.83	Joback Method
cpg	455.68	J/mol×K	808.31	Joback Method
cpg	468.40	J/mol×K	848.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25134218&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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