1,2,3,6-tetrahydromethylphthalic anhydride

Inchi: InChI=1S/C9H10O3/c1-5-2-3-6-7(4-5)9(11)12-8(6)10/h2,6-7H,3-4H2,1H3
InchiKey: OEMSKMUAMXLNKL-UHFFFAOYSA-N
Formula: C9H10O3
SMILES: CC1=CCC2C(=O)OC(=O)C2C1
Mol. weight [g/mol]: 166.17
CAS: 26590-20-5

Physical Properties

Property code	Value	Unit	Source
gf	-200.87	kJ/mol	Joback Method
hf	-463.06	kJ/mol	Joback Method
hfus	16.87	kJ/mol	Joback Method
hvap	49.93	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.042		Crippen Method
mcvol	120.660	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
tb	598.34	K	Joback Method
tc	849.13	K	Joback Method
tf	392.80	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.84	J/mol×K	598.34	Joback Method
cpg	335.09	J/mol×K	640.14	Joback Method
cpg	350.36	J/mol×K	681.94	Joback Method
cpg	364.62	J/mol×K	723.74	Joback Method
cpg	377.85	J/mol×K	765.54	Joback Method
cpg	390.03	J/mol×K	807.33	Joback Method
cpg	401.13	J/mol×K	849.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26590205&Units=SI

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