4-Methylphthalic anhydride

Other names: 1,3-Isobenzofurandione, 5-methyl-
5-methylisobenzofuran-1,3-dione
Inchi: InChI=1S/C9H6O3/c1-5-2-3-6-7(4-5)9(11)12-8(6)10/h2-4H,1H3
InchiKey: ZOXBWJMCXHTKNU-UHFFFAOYSA-N
Formula: C9H6O3
SMILES: Cc1ccc2c(c1)C(=O)OC2=O
Mol. weight [g/mol]: 162.14
CAS: 19438-61-0

Physical Properties

Property code	Value	Unit	Source
ea	1.19 ± 0.09	eV	NIST Webbook
gf	-144.79	kJ/mol	Joback Method
hf	-329.76	kJ/mol	Joback Method
hfus	16.39	kJ/mol	Joback Method
hvap	52.45	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	1.306		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	4124.99	kPa	Joback Method
tb	615.96	K	Joback Method
tc	873.64	K	Joback Method
tf	361.30	K	Solid-Liquid Phase Equilibria of the Ternary System (2-Naphthaldehyde + 4-Methylphthalic Anhydride + Ethyl Acetate) at (288.15, 298.15, and 308.15) K
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.44	J/mol×K	615.96	Joback Method

cpg	282.51	J/mol×K	658.91	Joback Method
cpg	293.82	J/mol×K	701.85	Joback Method
cpg	304.35	J/mol×K	744.80	Joback Method
cpg	314.08	J/mol×K	787.75	Joback Method
cpg	323.00	J/mol×K	830.69	Joback Method
cpg	331.09	J/mol×K	873.64	Joback Method

Sources

Solid-Liquid Phase Equilibria of the Ternary System (2-Naphthaldehyde + 4-Methylphthalic Anhydride + Ethyl Acetate) at (288.15, 298.15, and 308.15) K:	https://www.doi.org/10.1021/acs.jced.8b00170
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=C19438610&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
ea:	Electron affinity
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

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