Phenindione Me, #3

Inchi: InChI=1S/C16H12O2/c1-18-16-13-10-6-5-9-12(13)15(17)14(16)11-7-3-2-4-8-11/h2-10H,1
InchiKey: KYDYZFPREQVUJP-UHFFFAOYSA-N
Formula: C16H12O2
SMILES: COC1=C(c2ccccc2)C(=O)c2ccccc21
Mol. weight [g/mol]: 236.27

Physical Properties

Property code	Value	Unit	Source
gf	150.60	kJ/mol	Joback Method
hf	-53.92	kJ/mol	Joback Method
hfus	23.10	kJ/mol	Joback Method
hvap	64.92	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.398		Crippen Method
mcvol	181.060	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1481.00		NIST Webbook
rinpol	1481.00		NIST Webbook
tb	734.59	K	Joback Method
tc	993.26	K	Joback Method
tf	473.87	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.47	J/mol×K	734.59	Joback Method
cpg	498.61	J/mol×K	777.70	Joback Method
cpg	512.49	J/mol×K	820.81	Joback Method
cpg	525.18	J/mol×K	863.92	Joback Method
cpg	536.72	J/mol×K	907.03	Joback Method
cpg	547.19	J/mol×K	950.14	Joback Method
cpg	556.63	J/mol×K	993.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R40407&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