

P-quinone, p-ethoxyphenyl

Inchi:	InChI=1S/C14H12O3/c1-2-17-12-6-3-10(4-7-12)13-9-11(15)5-8-14(13)16/h3-9H,2H2,1H3
InchiKey:	UWAFVPYNCBNXAU-UHFFFAOYSA-N
Formula:	C14H12O3
SMILES:	CCOc1ccc(C2=CC(=O)C=CC2=O)cc1
Mol. weight [g/mol]:	228.24
CAS:	6276-62-6

Physical Properties

Property code	Value	Unit	Source
gf	-97.95	kJ/mol	Joback Method
hf	-336.10	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	62.58	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.177		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
tb	736.96	K	Joback Method
tc	994.75	K	Joback Method
tf	470.81	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.50	J/molxK	736.96	Joback Method
cpg	491.45	J/molxK	779.92	Joback Method
cpg	505.96	J/molxK	822.89	Joback Method
cpg	518.99	J/molxK	865.85	Joback Method
cpg	530.49	J/molxK	908.82	Joback Method
cpg	540.40	J/molxK	951.78	Joback Method
cpg	548.67	J/molxK	994.75	Joback Method

Sources

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=C6276626&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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