Retenequinone

Inchi: InChI=1S/C18H16O2/c1-10(2)12-7-8-13-14-6-4-5-11(3)16(14)18(20)17(19)15(13)9-12/h4
InchiKey: WVOVXOXRXQFTAS-UHFFFAOYSA-N
Formula: C18H16O2
SMILES: Cc1cccc2c1C(=O)C(=O)c1cc(C(C)C)ccc1-2
Mol. weight [g/mol]: 264.32
CAS: 5398-75-4

Physical Properties

Property code	Value	Unit	Source
chs	-9011.10	kJ/mol	NIST Webbook
chs	-9005.60	kJ/mol	NIST Webbook
gf	119.92	kJ/mol	Joback Method
hf	-169.05	kJ/mol	Joback Method
hfus	23.56	kJ/mol	Joback Method
hvap	71.02	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	4.164		Crippen Method
mcvol	209.240	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
tb	826.86	K	Joback Method
tc	1083.72	K	Joback Method
tf	542.68	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.06	J/mol×K	826.86	Joback Method
cpg	629.60	J/mol×K	869.67	Joback Method
cpg	643.80	J/mol×K	912.48	Joback Method
cpg	656.71	J/mol×K	955.29	Joback Method
cpg	668.36	J/mol×K	998.10	Joback Method
cpg	678.80	J/mol×K	1040.91	Joback Method
cpg	688.06	J/mol×K	1083.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5398754&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

chs:	Standard solid enthalpy of combustion
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