1H-Phenalen-1-one,9-ethoxy-

Inchi: InChI=1S/C15H12O2/c1-2-17-13-9-7-11-5-3-4-10-6-8-12(16)15(13)14(10)11/h3-9H,2H2,
InchiKey: PRACTAQKSAGYSP-UHFFFAOYSA-N
Formula: C15H12O2
SMILES: CCOc1ccc2cccc3c2c1C(=O)C=C3
Mol. weight [g/mol]: 224.25
CAS: 68217-42-5

Physical Properties

Property code	Value	Unit	Source
gf	136.42	kJ/mol	Joback Method
hf	-78.74	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	62.06	kJ/mol	Joback Method
ie	8.06 ± 0.04	eV	NIST Webbook
log10ws	-4.77		Crippen Method
logp	3.448		Crippen Method
mcvol	171.270	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
tb	704.01	K	Joback Method
tc	950.13	K	Joback Method
tf	468.88	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.29	J/mol×K	704.01	Joback Method
cpg	465.57	J/mol×K	745.03	Joback Method
cpg	478.84	J/mol×K	786.05	Joback Method
cpg	491.16	J/mol×K	827.07	Joback Method
cpg	502.59	J/mol×K	868.09	Joback Method
cpg	513.21	J/mol×K	909.11	Joback Method
cpg	523.08	J/mol×K	950.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68217425&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
ie:	Ionization energy
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