(E)-4-Phenylbut-3,4-epoxy-2-one

Inchi: InChI=1S/C10H10O2/c1-7(11)9-10(12-9)8-5-3-2-4-6-8/h2-6,9-10H,1H3/t9-,10-/m1/s1
InchiKey: IGCQIHCZUYCYAA-NXEZZACHSA-N
Formula: C10H10O2
SMILES: CC(=O)C1OC1c1ccccc1
Mol. weight [g/mol]: 162.19

Physical Properties

Property code	Value	Unit	Source
gf	-16.27	kJ/mol	Joback Method
hf	-205.32	kJ/mol	Joback Method
hfus	24.48	kJ/mol	Joback Method
hvap	50.99	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.716		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
rinpol	1340.00		NIST Webbook
tb	537.77	K	Joback Method
tc	767.59	K	Joback Method
tf	319.08	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.34	J/mol×K	537.77	Joback Method
cpg	306.92	J/mol×K	576.07	Joback Method
cpg	320.44	J/mol×K	614.38	Joback Method
cpg	332.96	J/mol×K	652.68	Joback Method
cpg	344.56	J/mol×K	690.98	Joback Method
cpg	355.28	J/mol×K	729.29	Joback Method
cpg	365.19	J/mol×K	767.59	Joback Method
dvisc	0.0022140	Pa×s	319.08	Joback Method
dvisc	0.0016082	Pa×s	355.53	Joback Method

dvisc	0.0012397	Pa×s	391.98	Joback Method
dvisc	0.0009989	Pa×s	428.43	Joback Method
dvisc	0.0008326	Pa×s	464.87	Joback Method
dvisc	0.0007127	Pa×s	501.32	Joback Method
dvisc	0.0006230	Pa×s	537.77	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R341278&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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