C11H10O2

Inchi: InChI=1S/C11H10O2/c12-11(13)9-5-4-8-10-6-2-1-3-7-10/h1-9H,(H,12,13)/b8-4+,9-5+
InchiKey: FEIQOMCWGDNMHM-KBXRYBNXSA-N
Formula: C11H10O2
SMILES: O=C(O)C=CC=Cc1ccccc1
Mol. weight [g/mol]: 174.20
CAS: 38446-98-9

Physical Properties

Property code	Value	Unit	Source
gf	48.85	kJ/mol	Joback Method
hf	-64.21	kJ/mol	Joback Method
hfus	24.38	kJ/mol	Joback Method
hvap	65.70	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.341		Crippen Method
mcvol	140.930	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
tb	632.13	K	Joback Method
tc	845.80	K	Joback Method
tf	340.74	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.55	J/mol×K	632.13	Joback Method
cpg	343.25	J/mol×K	667.74	Joback Method
cpg	353.19	J/mol×K	703.35	Joback Method
cpg	362.42	J/mol×K	738.97	Joback Method
cpg	371.01	J/mol×K	774.58	Joback Method
cpg	379.04	J/mol×K	810.19	Joback Method
cpg	386.55	J/mol×K	845.80	Joback Method
dvisc	0.0048140	Pa×s	340.74	Joback Method
dvisc	0.0014393	Pa×s	389.31	Joback Method

dvisc	0.0005625	Pa×s	437.87	Joback Method
dvisc	0.0002652	Pa×s	486.44	Joback Method
dvisc	0.0001433	Pa×s	535.00	Joback Method
dvisc	0.0000858	Pa×s	583.57	Joback Method
dvisc	0.0000556	Pa×s	632.13	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38446989&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume