

Acetic acid, 2-phenylcyclohexyl ester

Inchi:	InChI=1S/C14H18O2/c1-11(15)16-14-10-6-5-9-13(14)12-7-3-2-4-8-12/h2-4,7-8,13-14H,5
InchiKey:	OCJKSUSNMXDOGL-UHFFFAOYSA-N
Formula:	C14H18O2
SMILES:	CC(=O)OC1CCCCC1c1ccccc1
Mol. weight [g/mol]:	218.29
CAS:	63476-56-2

Physical Properties

Property code	Value	Unit	Source
gf	-37.77	kJ/mol	Joback Method
hf	-306.58	kJ/mol	Joback Method
hfus	21.75	kJ/mol	Joback Method
hvap	58.31	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.276		Crippen Method
mcvol	180.940	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
tb	637.57	K	Joback Method
tc	872.87	K	Joback Method
tf	349.26	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.59	J/molxK	637.57	Joback Method
cpg	507.71	J/molxK	676.79	Joback Method
cpg	526.40	J/molxK	716.00	Joback Method
cpg	543.69	J/molxK	755.22	Joback Method
cpg	559.63	J/molxK	794.44	Joback Method
cpg	574.24	J/molxK	833.65	Joback Method
cpg	587.56	J/molxK	872.87	Joback Method
dvisc	0.0022448	Paxs	349.26	Joback Method
dvisc	0.0011598	Paxs	397.31	Joback Method

dvisc	0.0006910	Paxs	445.36	Joback Method
dvisc	0.0004554	Paxs	493.41	Joback Method
dvisc	0.0003232	Paxs	541.47	Joback Method
dvisc	0.0002425	Paxs	589.52	Joback Method
dvisc	0.0001901	Paxs	637.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63476562&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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