1,4-Dioxane-2-carboxylic acid, 3-phenyl, ethyl ester

Inchi: InChI=1S/C13H16O4/c1-2-15-13(14)12-11(16-8-9-17-12)10-6-4-3-5-7-10/h3-7,11-12H,2,

InchiKey: AZBRMQHBGBXAAL-UHFFFAOYSA-N

Formula: C13H16O4

SMILES: CCOC(=O)C1OCCOC1c1ccccc1

Mol. weight [g/mol]: 236.26

Physical Properties

Property code	Value	Unit	Source
gf	-218.43	kJ/mol	Joback Method
hf	-549.94	kJ/mol	Joback Method
hfus	35.12	kJ/mol	Joback Method
hvap	65.10	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.706		Crippen Method
mcvol	178.590	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
tb	668.59	K	Joback Method
tc	902.33	K	Joback Method
tf	391.13	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.64	J/mol×K	668.59	Joback Method
cpg	517.35	J/mol×K	707.55	Joback Method
cpg	533.74	J/mol×K	746.50	Joback Method
cpg	548.83	J/mol×K	785.46	Joback Method
cpg	562.65	J/mol×K	824.42	Joback Method
cpg	575.22	J/mol×K	863.37	Joback Method
cpg	586.56	J/mol×K	902.33	Joback Method
dvisc	0.0020413	Pa×s	391.13	Joback Method

dvisc	0.0011061	Pa×s	437.37	Joback Method
dvisc	0.0006739	Pa×s	483.62	Joback Method
dvisc	0.0004477	Pa×s	529.86	Joback Method
dvisc	0.0003176	Pa×s	576.10	Joback Method
dvisc	0.0002371	Pa×s	622.35	Joback Method
dvisc	0.0001843	Pa×s	668.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R329421&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume