1,4-Dioxepane-2-carboxylic acid, 3-phenyl, ethyl ester, trans

Inchi: InChI=1S/C14H18O4/c1-2-16-14(15)13-12(17-9-6-10-18-13)11-7-4-3-5-8-11/h3-5,7-8,12-

InchiKey: JCVYDFPRMXWSHP-QWHCGFSZSA-N

Formula: C14H18O4

SMILES: CCOC(=O)C1OCCCOC1c1ccccc1

Mol. weight [g/mol]: 250.29

Physical Properties

Property code	Value	Unit	Source
gf	-222.11	kJ/mol	Joback Method
hf	-576.74	kJ/mol	Joback Method
hfus	35.61	kJ/mol	Joback Method
hvap	67.50	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.096		Crippen Method
mcvol	192.680	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1814.00		NIST Webbook
rinpol	1814.00		NIST Webbook
tb	695.74	K	Joback Method
tc	932.17	K	Joback Method
tf	398.88	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.58	J/mol×K	695.74	Joback Method
cpg	634.92	J/mol×K	892.76	Joback Method
cpg	621.94	J/mol×K	853.36	Joback Method
cpg	607.54	J/mol×K	813.95	Joback Method
cpg	591.69	J/mol×K	774.55	Joback Method
cpg	574.37	J/mol×K	735.14	Joback Method
cpg	646.48	J/mol×K	932.17	Joback Method
dvisc	0.0001198	Pa×s	695.74	Joback Method

dvisc	0.0001590	Pa×s	646.26	Joback Method
dvisc	0.0002213	Pa×s	596.79	Joback Method
dvisc	0.0003268	Pa×s	547.31	Joback Method
dvisc	0.0005215	Pa×s	497.83	Joback Method
dvisc	0.0009227	Pa×s	448.36	Joback Method
dvisc	0.0018807	Pa×s	398.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R329441&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

Latest version available from:
https://www.chemeo.com/cid/47-370-9/1-4-Dioxepane-2-carboxylic-acid-3-phenyl-ethyl-ester-trans.pdf
Generated by Cheméo on 2024-04-19 15:30:03.468519537 +0000 UTC m=+15829852.389096849.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.