trans-1-Carbethoxy-2-phenylcyclopropane

Other names:	trans-2-Phenylcyclopropanecarboxylic acid ethyl ester
	Ethyl trans-2-phenylcyclopropanecarboxylate
	Cyclopropanecarboxylic acid, 2-phenyl-, ethyl ester, trans-
	Cyclopropanecarboxylic acid, 2-phenyl-, ethyl ester, (1R,2R)-rel-
	1R,2R)-rel-2-Phenylcyclopropanecarboxylic acid ethyl ester
Inchi:	InChI=1S/C12H14O2/c1-2-14-12(13)11-8-10(11)9-6-4-3-5-7-9/h3-7,10-11H,2,8H2,1H3/t1
InchiKey:	SRGUIJLJERBBCM-WDEREUQCSA-N
Formula:	C12H14O2
SMILES:	CCOC(=O)C1CC1c1ccccc1
Mol. weight [g/mol]:	190.24
CAS:	946-39-4

Physical Properties

Property code	Value	Unit	Source
gf	-18.31	kJ/mol	Joback Method
hf	-246.82	kJ/mol	Joback Method
hfus	22.87	kJ/mol	Joback Method
hsub	96.90 ± 0.40	kJ/mol	NIST Webbook
hvap	53.34	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.353		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
tb	579.00	K	Joback Method
tc	799.97	K	Joback Method
tf	337.28	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.25	J/mol×K	579.00	Joback Method
cpg	397.58	J/mol×K	615.83	Joback Method
cpg	412.85	J/mol×K	652.66	Joback Method

cpg	427.10	J/mol×K	689.48	Joback Method
cpg	440.39	J/mol×K	726.31	Joback Method
cpg	452.77	J/mol×K	763.14	Joback Method
cpg	464.28	J/mol×K	799.97	Joback Method
dvisc	0.0018290	Pa×s	337.28	Joback Method
dvisc	0.0013003	Pa×s	377.57	Joback Method
dvisc	0.0009873	Pa×s	417.85	Joback Method
dvisc	0.0007868	Pa×s	458.14	Joback Method
dvisc	0.0006505	Pa×s	498.43	Joback Method
dvisc	0.0005533	Pa×s	538.71	Joback Method
dvisc	0.0004813	Pa×s	579.00	Joback Method

Sources

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=C946394&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
hsub: Enthalpy of sublimation 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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