

Cyclopropanecarboxylic acid, trans-2-phenyl-, butyl ester

Inchi:	InChI=1S/C14H18O2/c1-2-3-9-16-14(15)13-10-12(13)11-7-5-4-6-8-11/h4-8,12-13H,2-3,9
InchiKey:	CGIAMOFUTOLAEF-UHFFFAOYSA-N
Formula:	C14H18O2
SMILES:	CCCCOC(=O)C1CC1c1ccccc1
Mol. weight [g/mol]:	218.29

Physical Properties

Property code	Value	Unit	Source
gf	-1.47	kJ/mol	Joback Method
hf	-288.10	kJ/mol	Joback Method
hfus	28.05	kJ/mol	Joback Method
hvap	57.79	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.133		Crippen Method
mvol	180.940	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinpol	1716.00		NIST Webbook
rinpol	1716.00		NIST Webbook
tb	624.76	K	Joback Method
tc	838.14	K	Joback Method
tf	359.82	K	Joback Method
vc	0.692	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.60	J/molxK	624.76	Joback Method
cpg	498.95	J/molxK	660.32	Joback Method
cpg	515.21	J/molxK	695.89	Joback Method
cpg	530.43	J/molxK	731.45	Joback Method
cpg	544.66	J/molxK	767.01	Joback Method
cpg	557.96	J/molxK	802.58	Joback Method
cpg	570.36	J/molxK	838.14	Joback Method
dvisc	0.0019472	Paxs	359.82	Joback Method

dvisc	0.0013252	Paxs	403.98	Joback Method
dvisc	0.0009729	Paxs	448.13	Joback Method
dvisc	0.0007550	Paxs	492.29	Joback Method
dvisc	0.0006109	Paxs	536.45	Joback Method
dvisc	0.0005105	Paxs	580.60	Joback Method
dvisc	0.0004375	Paxs	624.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405994&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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