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

Inchi: InChI=1S/C17H22O2/c18-17(19-12-13-7-3-1-4-8-13)16-11-15(16)14-9-5-2-6-10-14/h2,5-

InchiKey: YMOFCEPOIRCUQY-UHFFFAOYSA-N

Formula: C17H22O2

SMILES: O=C(OCC1CCCCC1)C1CC1c1ccccc1

Mol. weight [g/mol]: 258.36

Physical Properties

Property code	Value	Unit	Source
gf	48.24	kJ/mol	Joback Method
hf	-295.70	kJ/mol	Joback Method
hfus	27.65	kJ/mol	Joback Method
hvap	64.90	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.914		Crippen Method
mcvol	212.350	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	2116.00		NIST Webbook
rinpol	2116.00		NIST Webbook
tb	712.95	K	Joback Method
tc	949.58	K	Joback Method
tf	401.01	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.83	J/mol×K	712.95	Joback Method
cpg	727.00	J/mol×K	910.14	Joback Method
cpg	711.86	J/mol×K	870.70	Joback Method
cpg	695.36	J/mol×K	831.26	Joback Method
cpg	677.42	J/mol×K	791.83	Joback Method
cpg	657.93	J/mol×K	752.39	Joback Method
cpg	740.85	J/mol×K	949.58	Joback Method
dvisc	0.0003827	Pa×s	712.95	Joback Method

dvisc	0.0004603	Pa×s	660.96	Joback Method
dvisc	0.0005714	Pa×s	608.97	Joback Method
dvisc	0.0007385	Pa×s	556.98	Joback Method
dvisc	0.0010063	Pa×s	504.99	Joback Method
dvisc	0.0014720	Pa×s	453.00	Joback Method
dvisc	0.0023764	Pa×s	401.01	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=U406842&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
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