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

Inchi: InChI=1S/C18H26O2/c1-3-5-9-14(4-2)13-20-18(19)17-12-16(17)15-10-7-6-8-11-15/h6-8,

InchiKey: KKKUGSXIQOSMKI-UHFFFAOYSA-N

Formula: C18H26O2

SMILES: CCCCC(CC)COC(=O)C1CC1c1ccccc1

Mol. weight [g/mol]: 274.40

Physical Properties

Property code	Value	Unit	Source
gf	29.77	kJ/mol	Joback Method
hf	-375.94	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	66.31	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.550		Crippen Method
mcvol	237.300	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	2042.00		NIST Webbook
rinpol	2042.00		NIST Webbook
tb	715.84	K	Joback Method
tc	921.00	K	Joback Method
tf	389.90	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.95	J/mol×K	715.84	Joback Method
cpg	717.79	J/mol×K	750.03	Joback Method
cpg	735.46	J/mol×K	784.23	Joback Method
cpg	752.04	J/mol×K	818.42	Joback Method
cpg	767.57	J/mol×K	852.61	Joback Method
cpg	782.11	J/mol×K	886.80	Joback Method
cpg	795.71	J/mol×K	921.00	Joback Method
dvisc	0.0021308	Pa×s	389.90	Joback Method

dvisc	0.0012576	Pa×s	444.22	Joback Method
dvisc	0.0008326	Pa×s	498.55	Joback Method
dvisc	0.0005977	Pa×s	552.87	Joback Method
dvisc	0.0004554	Pa×s	607.19	Joback Method
dvisc	0.0003627	Pa×s	661.52	Joback Method
dvisc	0.0002991	Pa×s	715.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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