

Cyclopropanecarboxylic acid, trans-2-phenyl-, 2-methylpent-3-yl ester

Inchi:	InChI=1S/C16H22O2/c1-4-15(11(2)3)18-16(17)14-10-13(14)12-8-6-5-7-9-12/h5-9,11,13-
InchiKey:	WLRXJBCJWGMBM-UHFFFAOYSA-N
Formula:	C16H22O2
SMILES:	CCC(OC(=O)C1CC1c1cccc1)C(C)C
Mol. weight [g/mol]:	246.34

Physical Properties

Property code	Value	Unit	Source
gf	10.49	kJ/mol	Joback Method
hf	-339.94	kJ/mol	Joback Method
hfus	26.18	kJ/mol	Joback Method
hvap	61.47	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.768		Crippen Method
mvol	209.120	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1777.00		NIST Webbook
rinpol	1777.00		NIST Webbook
tb	669.64	K	Joback Method
tc	884.28	K	Joback Method
tf	352.36	K	Joback Method
vc	0.791	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.48	J/molxK	669.64	Joback Method
cpg	607.27	J/molxK	705.41	Joback Method
cpg	624.84	J/molxK	741.19	Joback Method
cpg	641.27	J/molxK	776.96	Joback Method
cpg	656.59	J/molxK	812.73	Joback Method
cpg	670.88	J/molxK	848.51	Joback Method
cpg	684.20	J/molxK	884.28	Joback Method
dvisc	0.0025727	Paxs	352.36	Joback Method

dvisc	0.0014594	Paxs	405.24	Joback Method
dvisc	0.0009437	Paxs	458.12	Joback Method
dvisc	0.0006678	Paxs	511.00	Joback Method
dvisc	0.0005042	Paxs	563.88	Joback Method
dvisc	0.0003995	Paxs	616.76	Joback Method
dvisc	0.0003284	Paxs	669.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406836&Units=SI

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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