Cyclopropanecarboxylic acid, trans-2-phenyl-, dodec-2-en-1-yl ester

Inchi: InChI=1S/C22H32O2/c1-2-3-4-5-6-7-8-9-10-14-17-24-22(23)21-18-20(21)19-15-12-11-13

InchiKey: HTMWCOPTAPSNJJ-GXDHUFHOSA-N

Formula: C22H32O2

SMILES: CCCCCCCCCC=CCOC(=O)C1CC1c1ccccc1

Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	146.11	kJ/mol	Joback Method
hf	-336.00	kJ/mol	Joback Method
hfus	48.97	kJ/mol	Joback Method
hvap	75.56	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	6.030		Crippen Method
mcvol	289.360	ml/mol	McGowan Method
pc	1271.87	kPa	Joback Method
rinpol	2554.00		NIST Webbook
rinpol	2554.00		NIST Webbook
tb	811.96	K	Joback Method
tc	1014.41	K	Joback Method
tf	444.90	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.36	J/mol×K	811.96	Joback Method
cpg	991.01	J/mol×K	980.67	Joback Method
cpg	976.18	J/mol×K	946.93	Joback Method
cpg	960.47	J/mol×K	913.19	Joback Method
cpg	943.82	J/mol×K	879.44	Joback Method
cpg	926.14	J/mol×K	845.70	Joback Method
cpg	1005.04	J/mol×K	1014.41	Joback Method
dvisc	0.0001892	Pa×s	811.96	Joback Method

dvisc	0.0002312	Pa×s	750.78	Joback Method
dvisc	0.0002926	Pa×s	689.61	Joback Method
dvisc	0.0003879	Pa×s	628.43	Joback Method
dvisc	0.0005464	Pa×s	567.25	Joback Method
dvisc	0.0008362	Pa×s	506.08	Joback Method
dvisc	0.0014384	Pa×s	444.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U406848&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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