

Cyclopropanecarboxylic acid, trans-2-phenyl-, pentadec-5-yl ester

Inchi: InChI=1S/C25H40O2/c1-3-5-7-8-9-10-11-15-19-22(18-6-4-2)27-25(26)24-20-23(24)21-16
InchiKey: VBKFPQJGXNLF GK-UHFFFAOYSA-N
Formula: C25H40O2
SMILES: CCCCCCCCCC(CCCC)OC(=O)C1CC1c1ccccc1
Mol. weight [g/mol]: 372.58

Physical Properties

Property code	Value	Unit	Source
gf	88.71	kJ/mol	Joback Method
hf	-520.42	kJ/mol	Joback Method
hfus	53.02	kJ/mol	Joback Method
hvap	81.89	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	7.423		Crippen Method
mvol	335.930	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	2655.00		NIST Webbook
rinpol	2655.00		NIST Webbook
tb	876.00	K	Joback Method
tc	1078.33	K	Joback Method
tf	468.79	K	Joback Method
vc	1.302	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1117.57	J/molxK	876.00	Joback Method
cpg	1137.50	J/molxK	909.72	Joback Method
cpg	1156.20	J/molxK	943.44	Joback Method
cpg	1173.76	J/molxK	977.16	Joback Method
cpg	1190.24	J/molxK	1010.88	Joback Method
cpg	1205.72	J/molxK	1044.60	Joback Method
cpg	1220.28	J/molxK	1078.33	Joback Method
dvisc	0.0014187	Paxs	468.79	Joback Method

dvisc	0.0007545	Paxs	536.66	Joback Method
dvisc	0.0004624	Paxs	604.53	Joback Method
dvisc	0.0003129	Paxs	672.39	Joback Method
dvisc	0.0002274	Paxs	740.26	Joback Method
dvisc	0.0001744	Paxs	808.13	Joback Method
dvisc	0.0001393	Paxs	876.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406260&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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