Cyclopropanecarboxylic acid, trans-2-phenyl-, naphth-2-ylmethyl ester

Inchi: InChI=1S/C21H18O2/c22-21(20-13-19(20)17-7-2-1-3-8-17)23-14-15-10-11-16-6-4-5-9-18

InchiKey: RANFTECVFQGXMF-UHFFFAOYSA-N

Formula: C21H18O2

SMILES: O=C(OCc1ccc2ccccc2c1)C1CC1c1ccccc1

Mol. weight [g/mol]: 302.37

Physical Properties

Property code	Value	Unit	Source
gf	266.90	kJ/mol	Joback Method
hf	-16.45	kJ/mol	Joback Method
hfus	36.85	kJ/mol	Joback Method
hvap	77.95	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.687		Crippen Method
mcvol	236.350	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	2787.00		NIST Webbook
rinpol	2787.00		NIST Webbook
tb	835.56	K	Joback Method
tc	1086.65	K	Joback Method
tf	510.35	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.94	J/mol×K	835.56	Joback Method
cpg	725.08	J/mol×K	877.41	Joback Method
cpg	739.98	J/mol×K	919.26	Joback Method
cpg	753.79	J/mol×K	961.10	Joback Method
cpg	766.66	J/mol×K	1002.95	Joback Method
cpg	778.75	J/mol×K	1044.80	Joback Method
cpg	790.21	J/mol×K	1086.65	Joback Method
dvisc	0.0017616	Pa×s	510.35	Joback Method

dvisc	0.0013011	Pa×s	564.55	Joback Method
dvisc	0.0010134	Pa×s	618.75	Joback Method
dvisc	0.0008218	Pa×s	672.95	Joback Method
dvisc	0.0006875	Pa×s	727.16	Joback Method
dvisc	0.0005896	Pa×s	781.36	Joback Method
dvisc	0.0005158	Pa×s	835.56	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=U406850&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