

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

Inchi:	InChI=1S/C20H16O2/c21-20(19-13-18(19)15-7-2-1-3-8-15)22-17-11-10-14-6-4-5-9-16(14)
InchiKey:	MMVXWBSBJVZZLD-UHFFFAOYSA-N
Formula:	C20H16O2
SMILES:	O=C(Oc1ccc2ccccc2c1)C1CC1c1ccccc1
Mol. weight [g/mol]:	288.34

Physical Properties

Property code	Value	Unit	Source
gf	258.48	kJ/mol	Joback Method
hf	4.19	kJ/mol	Joback Method
hfus	34.26	kJ/mol	Joback Method
hvap	75.73	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.549		Crippen Method
mcvol	222.260	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	2695.00		NIST Webbook
tb	812.68	K	Joback Method
tc	1068.89	K	Joback Method
tf	499.08	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.77	J/molxK	812.68	Joback Method
cpg	721.31	J/molxK	1026.19	Joback Method
cpg	709.56	J/molxK	983.48	Joback Method
cpg	696.99	J/molxK	940.78	Joback Method
cpg	683.44	J/molxK	898.08	Joback Method
cpg	668.75	J/molxK	855.38	Joback Method
cpg	732.40	J/molxK	1068.89	Joback Method
dvisc	0.0005643	Paxs	812.68	Joback Method
dvisc	0.0006415	Paxs	760.41	Joback Method

dvisc	0.0007433	Paxs	708.15	Joback Method
dvisc	0.0008816	Paxs	655.88	Joback Method
dvisc	0.0010770	Paxs	603.61	Joback Method
dvisc	0.0013666	Paxs	551.35	Joback Method
dvisc	0.0018227	Paxs	499.08	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=U406885&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

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