

Cyclobutanecarboxylic acid, 2-naphthyl ester

Inchi:	InChI=1S/C15H14O2/c16-15(12-6-3-7-12)17-14-9-8-11-4-1-2-5-13(11)10-14/h1-2,4-5,8-1
InchiKey:	YGMZONJFWFDRPP-UHFFFAOYSA-N
Formula:	C15H14O2
SMILES:	O=C(Oc1ccc2ccccc2c1)C1CCC1
Mol. weight [g/mol]:	226.27

Physical Properties

Property code	Value	Unit	Source
gf	99.58	kJ/mol	Joback Method
hf	-114.96	kJ/mol	Joback Method
hfus	24.10	kJ/mol	Joback Method
hvap	62.80	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.545		Crippen Method
mcvol	175.570	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
rinsol	1944.00		NIST Webbook
tb	680.54	K	Joback Method
tc	925.32	K	Joback Method
tf	417.03	K	Joback Method
vc	0.662	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.64	J/molxK	680.54	Joback Method
cpg	541.06	J/molxK	884.52	Joback Method
cpg	529.33	J/molxK	843.72	Joback Method
cpg	516.63	J/molxK	802.93	Joback Method
cpg	502.85	J/molxK	762.13	Joback Method
cpg	487.89	J/molxK	721.34	Joback Method
cpg	551.92	J/molxK	925.32	Joback Method
dvisc	0.0004655	Paxs	680.54	Joback Method
dvisc	0.0005405	Paxs	636.62	Joback Method

dvisc	0.0006416	Paxs	592.70	Joback Method
dvisc	0.0007828	Paxs	548.78	Joback Method
dvisc	0.0009887	Paxs	504.87	Joback Method
dvisc	0.0013056	Paxs	460.95	Joback Method
dvisc	0.0018280	Paxs	417.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307443&Units=SI
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

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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