Cyclohexanecarboxylic acid, 2-naphthyl ester

Inchi: InChI=1S/C17H18O2/c18-17(14-7-2-1-3-8-14)19-16-11-10-13-6-4-5-9-15(13)12-16/h4-6,
InchiKey: DTJCAZMLSDVXEI-UHFFFAOYSA-N
Formula: C17H18O2
SMILES: O=C(Oc1ccc2ccccc2c1)C1CCCCC1
Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	92.22	kJ/mol	Joback Method
hf	-168.56	kJ/mol	Joback Method
hfus	25.08	kJ/mol	Joback Method
hvap	67.60	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.325		Crippen Method
mcvol	203.750	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
rinpol	2187.00		NIST Webbook
rinpol	2187.00		NIST Webbook
tb	734.84	K	Joback Method
tc	984.41	K	Joback Method
tf	432.53	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.50	J/mol×K	734.84	Joback Method
cpg	601.87	J/mol×K	776.44	Joback Method
cpg	618.70	J/mol×K	818.03	Joback Method
cpg	634.09	J/mol×K	859.63	Joback Method
cpg	648.13	J/mol×K	901.22	Joback Method
cpg	660.92	J/mol×K	942.82	Joback Method
cpg	672.54	J/mol×K	984.41	Joback Method
dvisc	0.0015212	Pa×s	432.53	Joback Method

dvisc	0.0009192	Pa×s	482.91	Joback Method
dvisc	0.0006109	Pa×s	533.30	Joback Method
dvisc	0.0004357	Pa×s	583.68	Joback Method
dvisc	0.0003279	Pa×s	634.07	Joback Method
dvisc	0.0002573	Pa×s	684.46	Joback Method
dvisc	0.0002087	Pa×s	734.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307709&Units=SI
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

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