1,2-Cyclohexanedicarboxylic acid, dicyclobutyl ester

Inchi: InChI=1S/C16H24O4/c17-15(19-11-5-3-6-11)13-9-1-2-10-14(13)16(18)20-12-7-4-8-12/h1

InchiKey: XBPOBMVRHJGQKA-UHFFFAOYSA-N

Formula: C16H24O4

SMILES: O=C(OC1CCC1)C1CCCCC1C(=O)OC1CCC1

Mol. weight [g/mol]: 280.36

Physical Properties

Property code	Value	Unit	Source
gf	-269.96	kJ/mol	Joback Method
hf	-695.91	kJ/mol	Joback Method
hfus	27.75	kJ/mol	Joback Method
hvap	69.81	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.984		Crippen Method
mcvol	218.600	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	2015.00		NIST Webbook
rinpol	2015.00		NIST Webbook
tb	754.96	K	Joback Method
tc	984.83	K	Joback Method
tf	446.38	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.40	J/mol×K	754.96	Joback Method
cpg	796.50	J/mol×K	946.52	Joback Method
cpg	781.89	J/mol×K	908.21	Joback Method
cpg	765.83	J/mol×K	869.90	Joback Method
cpg	748.27	J/mol×K	831.58	Joback Method
cpg	729.14	J/mol×K	793.27	Joback Method
cpg	809.73	J/mol×K	984.83	Joback Method
dvisc	0.0005023	Pa×s	754.96	Joback Method

dvisc	0.0005994	Pa×s	703.53	Joback Method
dvisc	0.0007355	Pa×s	652.10	Joback Method
dvisc	0.0009347	Pa×s	600.67	Joback Method
dvisc	0.0012423	Pa×s	549.24	Joback Method
dvisc	0.0017512	Pa×s	497.81	Joback Method
dvisc	0.0026718	Pa×s	446.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339758&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