1,1-CYCLOBUTANEDICARBOXYLIC ACID, DIETHYL ESTER

Other names: 1,1-Cyclobutanedicarboxylic acid, diethyl ester
Cyclobutane-1,1-dicarboxylic acid diethyl ester
Diethyl cyclobutane-1,1-dicarboxylate

Inchi: InChI=1S/C10H16O4/c1-3-13-8(11)10(6-5-7-10)9(12)14-4-2/h3-7H2,1-2H3

InchiKey: JPNJEJSZSMXWSV-UHFFFAOYSA-N

Formula: C10H16O4

SMILES: CCOC(=O)C1(C(=O)OCC)CCC1

Mol. weight [g/mol]: 200.23

Physical Properties

Property code	Value	Unit	Source
af	0.5352		Cheméo Relay (1.0)
gf	-391.36	kJ/mol	Joback Method
hf	-766.88	kJ/mol	Cheméo Relay (1.0)
hfus	16.97	kJ/mol	Joback Method
hvap	65.59	kJ/mol	Cheméo Relay (1.0)
ie	9.82	eV	Cheméo Relay (1.0)
log10ws	-2.35		Cheméo Relay (1.0)
logp	1.283		Crippen Method
mcvol	155.780	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
tb	497.20	K	NIST Webbook
tb	499.45 ± 1.50	K	NIST Webbook
tc	705.66	K	Cheméo Relay (1.0)
tf	297.82	K	Cheméo Relay (1.0)
vc	0.567	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.45	J/mol×K	592.03	Joback Method
cpg	414.60	J/mol×K	626.26	Joback Method
cpg	428.01	J/mol×K	660.49	Joback Method
cpg	440.77	J/mol×K	694.72	Joback Method

cpg	452.95	J/mol×K	728.95	Joback Method
cpg	464.66	J/mol×K	763.18	Joback Method
cpg	475.96	J/mol×K	797.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.20	K	1.60	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3779291&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume