

Diethyl 1,1-cyclobutanedicarboxylate

Other names:	Cyclobutane-1,1-dicarboxylic acid diethyl ester Diethyl cyclobutane-1,1-dicarboxylate 1,1-Cyclobutanedicarboxylic acid, diethyl ester
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
CAS:	3779-29-1

Physical Properties

Property code	Value	Unit	Source
gf	-391.36	kJ/mol	Joback Method
hf	-657.45	kJ/mol	Joback Method
hfus	16.97	kJ/mol	Joback Method
hvap	55.10	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.283		Crippen Method
mcvol	155.780	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
tb	499.45 ± 1.50	K	NIST Webbook
tb	497.20	K	NIST Webbook
tc	797.41	K	Joback Method
tf	385.10	K	Joback Method
vc	0.591	m3/kmol	Joback Method

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

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

Legend

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
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

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