

Cyclobutanecarboxylic acid, 2-dimethylamino-3,3-dimethyl, methyl ester

Inchi:	InChI=1S/C10H19NO2/c1-10(2)6-7(9(12)13-5)8(10)11(3)4/h7-8H,6H2,1-5H3
InchiKey:	CHHNTSCHGQVFAT-UHFFFAOYSA-N
Formula:	C10H19NO2
SMILES:	COC(=O)C1CC(C)(C)C1N(C)C
Mol. weight [g/mol]:	185.26
CAS:	3854-82-8

Physical Properties

Property code	Value	Unit	Source
gf	-62.08	kJ/mol	Joback Method
hf	-385.80	kJ/mol	Joback Method
hfus	19.34	kJ/mol	Joback Method
hvap	47.37	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	1.136		Crippen Method
mcvol	158.320	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
tb	518.84	K	Joback Method
tc	714.87	K	Joback Method
tf	336.93	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.68	J/molxK	518.84	Joback Method
cpg	407.93	J/molxK	551.51	Joback Method
cpg	424.22	J/molxK	584.18	Joback Method
cpg	439.64	J/molxK	616.85	Joback Method
cpg	454.25	J/molxK	649.53	Joback Method
cpg	468.16	J/molxK	682.20	Joback Method
cpg	481.43	J/molxK	714.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3854828&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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