1-Cyclobutenecarboxylic acid, 3,3-dimethyl ethyl ester

Inchi: InChI=1S/C9H14O2/c1-4-11-8(10)7-5-9(2,3)6-7/h5H,4,6H2,1-3H3
InchiKey: JWFAARURPAFBBJ-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CCOC(=O)C1=CC(C)(C)C1
Mol. weight [g/mol]: 154.21
CAS: 37676-92-9

Physical Properties

Property code	Value	Unit	Source
gf	-145.53	kJ/mol	Joback Method
hf	-345.70	kJ/mol	Joback Method
hfus	12.42	kJ/mol	Joback Method
hvap	44.67	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.906		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
tb	497.00	K	Joback Method
tc	701.94	K	Joback Method
tf	314.95	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.41	J/mol×K	497.00	Joback Method
cpg	305.93	J/mol×K	531.16	Joback Method
cpg	318.62	J/mol×K	565.31	Joback Method
cpg	330.55	J/mol×K	599.47	Joback Method
cpg	341.83	J/mol×K	633.63	Joback Method
cpg	352.55	J/mol×K	667.78	Joback Method
cpg	362.79	J/mol×K	701.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37676929&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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume