

ETHYL 2,2,3,3-TETRAMETHYLCYCLOPROPANE-CARBOXYLATE

Inchi: InChI=1S/C10H18O2/c1-6-12-8(11)7-9(2,3)10(7,4)5/h7H,6H2,1-5H3
InchiKey: JGWIOJNKGNJJLE-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CCOC(=O)C1C(C)(C)C1(C)C
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
af	0.4096		Cheméo Relay (1.0)
gf	-166.25	kJ/mol	Joback Method
hf	-482.86	kJ/mol	Cheméo Relay (1.0)
hfus	12.12	kJ/mol	Joback Method
hvap	55.82	kJ/mol	Cheméo Relay (1.0)
ie	9.11	eV	Cheméo Relay (1.0)
log10ws	-2.44		Cheméo Relay (1.0)
logp	2.232		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
tb	441.93	K	Cheméo Relay (1.0)
tc	679.50	K	Cheméo Relay (1.0)
tf	328.92	K	Cheméo Relay (1.0)
vc	0.505	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.76	J/mol×K	502.37	Joback Method
cpg	371.44	J/mol×K	535.60	Joback Method
cpg	386.08	J/mol×K	568.83	Joback Method
cpg	399.84	J/mol×K	602.06	Joback Method
cpg	412.88	J/mol×K	635.30	Joback Method
cpg	425.32	J/mol×K	668.53	Joback Method
cpg	437.34	J/mol×K	701.76	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	349.70	K	2.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C771108&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

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

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