

(CH3)2C(C2H5)OOC(CH3)2C2H5

Other names: (CH3)2C(C2H5)OOC(CH3)2C2H5
Inchi: InChI=1S/C10H22O2/c1-7-9(3,4)11-12-10(5,6)8-2/h7-8H2,1-6H3
InchiKey: JJRDRFZYKKFYMO-UHFFFAOYSA-N
Formula: C10H22O2
SMILES: CCC(C)(C)OOC(C)(C)CC
Mol. weight [g/mol]: 174.28

Physical Properties

Property code	Value	Unit	Source
af	0.4990		Cheméo Relay (1.0)
chl	-6479.80	kJ/mol	NIST Webbook
gf	-171.00	kJ/mol	Joback Method
hf	-388.11	kJ/mol	Cheméo Relay (1.0)
hfl	-599.60	kJ/mol	NIST Webbook
hfus	9.20	kJ/mol	Joback Method
hvap	51.16	kJ/mol	Cheméo Relay (1.0)
ie	8.64	eV	Cheméo Relay (1.0)
log10ws	-2.79		Cheméo Relay (1.0)
logp	3.312		Crippen Method
mcvol	163.500	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
tb	444.54	K	Cheméo Relay (1.0)
tc	620.72	K	Cheméo Relay (1.0)
tf	255.94	K	Cheméo Relay (1.0)
vc	0.649	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.05	J/mol×K	466.58	Joback Method
cpg	391.08	J/mol×K	497.01	Joback Method
cpg	407.31	J/mol×K	527.43	Joback Method
cpg	422.77	J/mol×K	557.86	Joback Method
cpg	437.48	J/mol×K	588.28	Joback Method

cpg	451.46	J/mol×K	618.71	Joback Method
cpg	464.75	J/mol×K	649.13	Joback Method
dvisc	0.0063620	Pa×s	251.76	Joback Method
dvisc	0.0023929	Pa×s	287.56	Joback Method
dvisc	0.0011176	Pa×s	323.37	Joback Method
dvisc	0.0006075	Pa×s	359.17	Joback Method
dvisc	0.0003688	Pa×s	394.97	Joback Method
dvisc	0.0002433	Pa×s	430.78	Joback Method
dvisc	0.0001711	Pa×s	466.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	331.70	K	1.90	NIST Webbook
tbrp	331.60	K	1.90	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C10508095&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

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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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