DIETHYL ISOPROPYLMETHYLMALONATE

Other names: Diethyl isopropylmethylmalonate
Inchi: InChI=1S/C11H20O4/c1-6-14-9(12)11(5,8(3)4)10(13)15-7-2/h8H,6-7H2,1-5H3
InchiKey: NQSVPQIOJRYMGQ-UHFFFAOYSA-N
Formula: C11H20O4
SMILES: CCOC(=O)C(C)(C(=O)OCC)C(C)C
Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
af	0.5430		Cheméo Relay (1.0)
gf	-425.70	kJ/mol	Joback Method
hf	-886.87	kJ/mol	Cheméo Relay (1.0)
hfus	18.88	kJ/mol	Joback Method
hvap	62.80	kJ/mol	Cheméo Relay (1.0)
ie	9.61	eV	Cheméo Relay (1.0)
log10ws	-2.21		Cheméo Relay (1.0)
logp	1.775		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
tb	475.52	K	Cheméo Relay (1.0)
tc	675.84	K	Cheméo Relay (1.0)
tf	257.92	K	Cheméo Relay (1.0)
vc	0.647	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.59	J/mol×K	599.99	Joback Method
cpg	483.45	J/mol×K	631.83	Joback Method
cpg	497.56	J/mol×K	663.67	Joback Method
cpg	510.92	J/mol×K	695.51	Joback Method
cpg	523.56	J/mol×K	727.36	Joback Method
cpg	535.49	J/mol×K	759.20	Joback Method
cpg	546.72	J/mol×K	791.04	Joback Method

dvisc	0.0025750	Pa×s	345.47	Joback Method
dvisc	0.0012195	Pa×s	387.89	Joback Method
dvisc	0.0006692	Pa×s	430.31	Joback Method
dvisc	0.0004090	Pa×s	472.73	Joback Method
dvisc	0.0002711	Pa×s	515.15	Joback Method
dvisc	0.0001913	Pa×s	557.57	Joback Method
dvisc	0.0001418	Pa×s	599.99	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58447691&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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