Propanedioic acid, propyl-, diethyl ester

Other names:	Malonic acid, propyl-, diethyl ester
	Propanedioic acid, propyl-, diethyl ester
	Propylmalonic acid diethyl ester
Inchi:	InChI=1S/C10H18O4/c1-4-7-8(9(11)13-5-2)10(12)14-6-3/h8H,4-7H2,1-3H3
InchiKey:	GRRSDGHTSMJICM-UHFFFAOYSA-N
Formula:	C10H18O4
SMILES:	CCCC(C(=O)OCC)C(=O)OCC
Mol. weight [g/mol]:	202.25

Physical Properties

Property code	Value	Unit	Source
af	0.5916		Cheméo Relay (1.0)
gf	-436.96	kJ/mol	Joback Method
hf	-883.11	kJ/mol	Cheméo Relay (1.0)
hfus	23.71	kJ/mol	Joback Method
hvap	68.55	kJ/mol	Cheméo Relay (1.0)
ie	9.76	eV	Cheméo Relay (1.0)
log10ws	-2.04		Cheméo Relay (1.0)
logp	1.529		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
tb	495.09	K	Cheméo Relay (1.0)
tc	665.30	K	Cheméo Relay (1.0)
tf	216.46	K	Cheméo Relay (1.0)
vc	0.618	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.07	J/mol×K	580.34	Joback Method
cpg	429.55	J/mol×K	610.90	Joback Method
cpg	442.48	J/mol×K	641.47	Joback Method
cpg	454.83	J/mol×K	672.03	Joback Method
cpg	466.62	J/mol×K	702.60	Joback Method

cpg	477.83	J/mol×K	733.16	Joback Method
cpg	488.46	J/mol×K	763.73	Joback Method
dvisc	0.0024229	Pa×s	331.78	Joback Method
dvisc	0.0012300	Pa×s	373.21	Joback Method
dvisc	0.0007150	Pa×s	414.63	Joback Method
dvisc	0.0004587	Pa×s	456.06	Joback Method
dvisc	0.0003168	Pa×s	497.49	Joback Method
dvisc	0.0002316	Pa×s	538.91	Joback Method
dvisc	0.0001771	Pa×s	580.34	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2163486&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

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