DIETHYL DIBUTYLMALONATE

Other names: Malonic acid, dibutyl-, diethyl ester
Diethyl dibutylmalonate
Inchi: InChI=1S/C15H28O4/c1-5-9-11-15(12-10-6-2,13(16)18-7-3)14(17)19-8-4/h5-12H2,1-4H3
InchiKey: WHKKUUPZLWUOIW-UHFFFAOYSA-N
Formula: C15H28O4
SMILES: CCCCC(CCCC)(C(=O)OCC)C(=O)OCC
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
hf	-942.37	kJ/mol	Cheméo Relay (1.0)
hfus	32.77	kJ/mol	Joback Method
hvap	71.90	kJ/mol	Cheméo Relay (1.0)
ie	9.38	eV	Cheméo Relay (1.0)
log10ws	-3.87		Cheméo Relay (1.0)
logp	3.479		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
tb	550.43	K	Cheméo Relay (1.0)
tc	723.29	K	Cheméo Relay (1.0)
tf	249.99	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.64	J/mol×K	691.95	Joback Method
cpg	766.12	J/mol×K	874.06	Joback Method
cpg	753.71	J/mol×K	843.71	Joback Method
cpg	740.53	J/mol×K	813.36	Joback Method
cpg	726.55	J/mol×K	783.00	Joback Method
cpg	711.75	J/mol×K	752.65	Joback Method
cpg	696.12	J/mol×K	722.30	Joback Method
dvisc	0.0002466	Pa×s	548.75	Joback Method
dvisc	0.0000891	Pa×s	691.95	Joback Method

dvisc	0.0001190	Pa×s	644.22	Joback Method
dvisc	0.0001664	Pa×s	596.48	Joback Method
dvisc	0.0014014	Pa×s	405.55	Joback Method
dvisc	0.0003941	Pa×s	501.02	Joback Method
dvisc	0.0006952	Pa×s	453.28	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C596758&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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