2-OCTYLMALONIC ACID, DIETHYL ESTER

Other names: Malonic acid, octyl-, diethyl ester
Propanedioic acid, octyl-, diethyl ester
Inchi: InChI=1S/C15H28O4/c1-4-7-8-9-10-11-12-13(14(16)18-5-2)15(17)19-6-3/h13H,4-12H2,1
InchiKey: YZYBVYGISZANLI-UHFFFAOYSA-N
Formula: C15H28O4
SMILES: CCCCCCCCC(C(=O)OCC)C(=O)OCC
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
af	0.7779		Cheméo Relay (1.0)
gf	-394.86	kJ/mol	Joback Method
hf	-977.58	kJ/mol	Cheméo Relay (1.0)
hfus	36.66	kJ/mol	Joback Method
hvap	85.37	kJ/mol	Cheméo Relay (1.0)
ie	9.59	eV	Cheméo Relay (1.0)
log10ws	-4.06		Cheméo Relay (1.0)
logp	3.479		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	1703.00		NIST Webbook
rinpol	1703.00		NIST Webbook
tb	559.88	K	Cheméo Relay (1.0)
tc	732.91	K	Cheméo Relay (1.0)
tf	240.27	K	Cheméo Relay (1.0)
vc	0.893	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.76	J/mol×K	694.74	Joback Method
cpg	694.10	J/mol×K	724.41	Joback Method
cpg	709.65	J/mol×K	754.07	Joback Method
cpg	724.41	J/mol×K	783.74	Joback Method

cpg	738.39	J/mol×K	813.41	Joback Method
cpg	751.59	J/mol×K	843.08	Joback Method
cpg	764.02	J/mol×K	872.74	Joback Method
dvisc	0.0016719	Pa×s	388.13	Joback Method
dvisc	0.0007909	Pa×s	439.23	Joback Method
dvisc	0.0004373	Pa×s	490.33	Joback Method
dvisc	0.0002704	Pa×s	541.43	Joback Method
dvisc	0.0001817	Pa×s	592.54	Joback Method
dvisc	0.0001300	Pa×s	643.64	Joback Method
dvisc	0.0000977	Pa×s	694.74	Joback Method

Sources

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=C1472851&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume