Dioctyl malonate

Other names: Propanedioic acid, dioctyl ester
Inchi: InChI=1S/C19H36O4/c1-3-5-7-9-11-13-15-22-18(20)17-19(21)23-16-14-12-10-8-6-4-2/h3
InchiKey: DTVMXQFQTCJMOR-UHFFFAOYSA-N
Formula: C19H36O4
SMILES: CCCCCCCCOC(=O)CC(=O)OCCCCCCCC
Mol. weight [g/mol]: 328.49
CAS: 16958-88-6

Physical Properties

Property code	Value	Unit	Source
gf	-358.74	kJ/mol	Joback Method
hf	-925.09	kJ/mol	Joback Method
hfus	50.54	kJ/mol	Joback Method
hvap	76.20	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	5.184		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1149.10	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2108.00		NIST Webbook
rinpol	2168.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	786.70	K	Joback Method
tc	967.58	K	Joback Method
tf	448.21	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.90	J/mol×K	786.70	Joback Method
cpg	926.73	J/mol×K	816.85	Joback Method
cpg	943.58	J/mol×K	846.99	Joback Method
cpg	959.47	J/mol×K	877.14	Joback Method

cpg	974.42	J/mol×K	907.29	Joback Method
cpg	988.43	J/mol×K	937.43	Joback Method
cpg	1001.52	J/mol×K	967.58	Joback Method
dvisc	0.0009350	Pa×s	448.21	Joback Method
dvisc	0.0004609	Pa×s	504.63	Joback Method
dvisc	0.0002619	Pa×s	561.04	Joback Method
dvisc	0.0001650	Pa×s	617.46	Joback Method
dvisc	0.0001123	Pa×s	673.87	Joback Method
dvisc	0.0000812	Pa×s	730.29	Joback Method
dvisc	0.0000614	Pa×s	786.70	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16958886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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