Diglycolic acid, di(octyl) ester

Other names: dioctyl 2,2'-oxydiacetate
dioctyl diglycolate
Inchi: InChI=1S/C20H38O5/c1-3-5-7-9-11-13-15-24-19(21)17-23-18-20(22)25-16-14-12-10-8-6
InchiKey: RIDUWSCSWADNHH-UHFFFAOYSA-N
Formula: C20H38O5
SMILES: CCCCCCCCOC(=O)COCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 358.51

Physical Properties

Property code	Value	Unit	Source
gf	-455.32	kJ/mol	Joback Method
hf	-1077.95	kJ/mol	Joback Method
hfus	54.32	kJ/mol	Joback Method
hvap	80.84	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.810		Crippen Method
mcvol	313.410	ml/mol	McGowan Method
pc	1065.87	kPa	Joback Method
rinpol	3004.00		NIST Webbook
rinpol	3004.00		NIST Webbook
tb	832.00	K	Joback Method
tc	1019.41	K	Joback Method
tf	481.71	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.84	J/mol×K	832.00	Joback Method
cpg	1018.88	J/mol×K	863.24	Joback Method
cpg	1035.80	J/mol×K	894.47	Joback Method
cpg	1051.59	J/mol×K	925.71	Joback Method
cpg	1066.26	J/mol×K	956.94	Joback Method
cpg	1079.84	J/mol×K	988.18	Joback Method

cpg	1092.31	J/mol×K	1019.41	Joback Method
dvisc	0.0005736	Pa×s	481.71	Joback Method
dvisc	0.0002891	Pa×s	540.09	Joback Method
dvisc	0.0001666	Pa×s	598.47	Joback Method
dvisc	0.0001059	Pa×s	656.86	Joback Method
dvisc	0.0000725	Pa×s	715.24	Joback Method
dvisc	0.0000525	Pa×s	773.62	Joback Method
dvisc	0.0000398	Pa×s	832.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382116&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
New Highly CO2-Philic Diglycolic Acid Esters: Synthesis and Solubility in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je900893e
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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