1,2-Dioctanoin

Inchi: InChI=1S/C19H36O5/c1-3-5-7-9-11-13-18(21)23-16-17(15-20)24-19(22)14-12-10-8-6-4-2
InchiKey: ZQBULZYTDGUSSK-UHFFFAOYSA-N
Formula: C19H36O5
SMILES: CCCCCCCC(=O)OCC(CO)OC(=O)CCCCCCC
Mol. weight [g/mol]: 344.49
CAS: 1069-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-498.00	kJ/mol	Joback Method
hf	-1082.60	kJ/mol	Joback Method
hfus	51.10	kJ/mol	Joback Method
hvap	92.49	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.155		Crippen Method
mcvol	299.320	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	2359.30		NIST Webbook
rinpol	2359.30		NIST Webbook
tb	878.44	K	Joback Method
tc	1075.60	K	Joback Method
tf	494.03	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	979.17	J/mol×K	878.44	Joback Method
cpg	995.44	J/mol×K	911.30	Joback Method
cpg	1010.59	J/mol×K	944.16	Joback Method
cpg	1024.63	J/mol×K	977.02	Joback Method
cpg	1037.59	J/mol×K	1009.88	Joback Method
cpg	1049.49	J/mol×K	1042.74	Joback Method
cpg	1060.34	J/mol×K	1075.60	Joback Method

dvisc	0.0004866	Pa×s	494.03	Joback Method
dvisc	0.0001674	Pa×s	558.10	Joback Method
dvisc	0.0000717	Pa×s	622.17	Joback Method
dvisc	0.0000360	Pa×s	686.24	Joback Method
dvisc	0.0000203	Pa×s	750.30	Joback Method
dvisc	0.0000126	Pa×s	814.37	Joback Method
dvisc	0.0000083	Pa×s	878.44	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1069870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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