di-(2-Methoxybutyl)azelate

Inchi: InChI=1S/C19H36O6/c1-5-16(22-3)14-24-18(20)12-10-8-7-9-11-13-19(21)25-15-17(6-2)2
InchiKey: XQBSLZDCJGTJFL-UHFFFAOYSA-N
Formula: C19H36O6
SMILES: CCC(COC(=O)CCCCCCCC(=O)OCC(CC)OC)OC
Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-573.62	kJ/mol	Joback Method
hf	-1200.09	kJ/mol	Joback Method
hfus	45.87	kJ/mol	Joback Method
hvap	80.24	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.654		Crippen Method
mcvol	305.190	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
rinpol	2048.00		NIST Webbook
rinpol	2048.00		NIST Webbook
tb	830.66	K	Joback Method
tc	1019.18	K	Joback Method
tf	462.67	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.42	J/mol×K	830.66	Joback Method
cpg	989.90	J/mol×K	862.08	Joback Method
cpg	1006.21	J/mol×K	893.50	Joback Method
cpg	1021.33	J/mol×K	924.92	Joback Method
cpg	1035.27	J/mol×K	956.34	Joback Method
cpg	1048.03	J/mol×K	987.76	Joback Method
cpg	1059.59	J/mol×K	1019.18	Joback Method
dvisc	0.0005940	Pa×s	462.67	Joback Method

dvisc	0.0002674	Pa×s	524.00	Joback Method
dvisc	0.0001422	Pa×s	585.33	Joback Method
dvisc	0.0000853	Pa×s	646.66	Joback Method
dvisc	0.0000559	Pa×s	708.00	Joback Method
dvisc	0.0000392	Pa×s	769.33	Joback Method
dvisc	0.0000289	Pa×s	830.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R542124&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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