

di-(1-Methyl-2-methoxybutyl)azelate

Inchi:	InChI=1S/C19H36O6/c1-14(22-5)16(3)24-18(20)12-10-8-7-9-11-13-19(21)25-17(4)15(2)2
InchiKey:	IDFWZXJFXXOTQU-UHFFFAOYSA-N
Formula:	C19H36O6
SMILES:	COC(C)C(C)OC(=O)CCCCCCCC(=O)OC(C)C(C)OC
Mol. weight [g/mol]:	360.49

Physical Properties

Property code	Value	Unit	Source
gf	-578.50	kJ/mol	Joback Method
hf	-1210.65	kJ/mol	Joback Method
hfus	38.82	kJ/mol	Joback Method
hvap	79.47	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.650		Crippen Method
mcvol	305.190	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinpol	2088.00		NIST Webbook
tb	829.78	K	Joback Method
tc	1019.91	K	Joback Method
tf	432.67	K	Joback Method
vc	1.159	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	973.40	J/molxK	829.78	Joback Method
cpg	991.02	J/molxK	861.47	Joback Method
cpg	1007.43	J/molxK	893.16	Joback Method
cpg	1022.62	J/molxK	924.85	Joback Method
cpg	1036.59	J/molxK	956.53	Joback Method
cpg	1049.33	J/molxK	988.22	Joback Method
cpg	1060.83	J/molxK	1019.91	Joback Method
dvisc	0.0008685	Paxs	432.67	Joback Method
dvisc	0.0003224	Paxs	498.86	Joback Method

dvisc	0.0001510	Paxs	565.04	Joback Method
dvisc	0.0000829	Paxs	631.22	Joback Method
dvisc	0.0000510	Paxs	697.41	Joback Method
dvisc	0.0000341	Paxs	763.60	Joback Method
dvisc	0.0000243	Paxs	829.78	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=R541829&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

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