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

Inchi: InChI=1S/C16H30O6/c1-11(19-5)13(3)21-15(17)9-7-8-10-16(18)22-14(4)12(2)20-6/h11-1
InchiKey: CZSSMCJAVMVEBB-UHFFFAOYSA-N
Formula: C16H30O6
SMILES: COC(C)C(C)OC(=O)CCCCC(=O)OC(C)C(C)OC
Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-603.76	kJ/mol	Joback Method
hf	-1148.73	kJ/mol	Joback Method
hfus	31.05	kJ/mol	Joback Method
hvap	72.79	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.480		Crippen Method
mcvol	262.920	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
rinpol	1790.00		NIST Webbook
tb	761.14	K	Joback Method
tc	946.78	K	Joback Method
tf	398.86	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.69	J/mol×K	761.14	Joback Method
cpg	869.60	J/mol×K	915.84	Joback Method
cpg	856.85	J/mol×K	884.90	Joback Method
cpg	843.08	J/mol×K	853.96	Joback Method
cpg	828.29	J/mol×K	823.02	Joback Method
cpg	812.49	J/mol×K	792.08	Joback Method
cpg	881.30	J/mol×K	946.78	Joback Method
dvisc	0.0000383	Pa×s	761.14	Joback Method
dvisc	0.0000535	Pa×s	700.76	Joback Method

dvisc	0.0000795	Pa×s	640.38	Joback Method
dvisc	0.0001284	Pa×s	580.00	Joback Method
dvisc	0.0002319	Pa×s	519.62	Joback Method
dvisc	0.0004890	Pa×s	459.24	Joback Method
dvisc	0.0012927	Pa×s	398.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541814&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
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