di-(3-Methoxybutyl)adipate

Inchi: InChI=1S/C16H30O6/c1-13(19-3)9-11-21-15(17)7-5-6-8-16(18)22-12-10-14(2)20-4/h13-1
InchiKey: ATLKKGZUMZYLGA-UHFFFAOYSA-N
Formula: C16H30O6
SMILES: COC(C)CCOC(=O)CCCCC(=O)OCCC(C)OC
Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-598.88	kJ/mol	Joback Method
hf	-1138.17	kJ/mol	Joback Method
hfus	38.10	kJ/mol	Joback Method
hvap	73.57	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.483		Crippen Method
mcvol	262.920	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	2038.00		NIST Webbook
tb	762.02	K	Joback Method
tc	944.23	K	Joback Method
tf	428.86	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.68	J/mol×K	762.02	Joback Method
cpg	811.15	J/mol×K	792.39	Joback Method
cpg	826.67	J/mol×K	822.76	Joback Method
cpg	841.24	J/mol×K	853.13	Joback Method
cpg	854.84	J/mol×K	883.50	Joback Method
cpg	867.47	J/mol×K	913.86	Joback Method
cpg	879.11	J/mol×K	944.23	Joback Method
dvisc	0.0008446	Pa×s	428.86	Joback Method
dvisc	0.0003918	Pa×s	484.39	Joback Method

dvisc	0.0002129	Pa×s	539.91	Joback Method
dvisc	0.0001296	Pa×s	595.44	Joback Method
dvisc	0.0000859	Pa×s	650.97	Joback Method
dvisc	0.0000607	Pa×s	706.49	Joback Method
dvisc	0.0000451	Pa×s	762.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R542208&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