di-(3-Methoxybutyl)suberate

Inchi: InChI=1S/C18H34O6/c1-15(21-3)11-13-23-17(19)9-7-5-6-8-10-18(20)24-14-12-16(2)22-4
InchiKey: XGQWLZVUXLGDFS-UHFFFAOYSA-N
Formula: C18H34O6
SMILES: COC(C)CCOC(=O)CCCCCCC(=O)OCCC(C)OC
Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-582.04	kJ/mol	Joback Method
hf	-1179.45	kJ/mol	Joback Method
hfus	43.28	kJ/mol	Joback Method
hvap	78.02	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.263		Crippen Method
mcvol	291.100	ml/mol	McGowan Method
pc	1212.36	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	807.78	K	Joback Method
tc	993.49	K	Joback Method
tf	451.40	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.35	J/mol×K	807.78	Joback Method
cpg	929.50	J/mol×K	838.73	Joback Method
cpg	945.56	J/mol×K	869.68	Joback Method
cpg	960.52	J/mol×K	900.64	Joback Method
cpg	974.39	J/mol×K	931.59	Joback Method
cpg	987.14	J/mol×K	962.54	Joback Method
cpg	998.78	J/mol×K	993.49	Joback Method
dvisc	0.0006705	Pa×s	451.40	Joback Method

dvisc	0.0003047	Pa×s	510.80	Joback Method
dvisc	0.0001632	Pa×s	570.19	Joback Method
dvisc	0.0000983	Pa×s	629.59	Joback Method
dvisc	0.0000647	Pa×s	688.99	Joback Method
dvisc	0.0000454	Pa×s	748.38	Joback Method
dvisc	0.0000336	Pa×s	807.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R542273&Units=SI

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