di-(2-Methoxybutyl)sebacate

Inchi: InChI=1S/C20H38O6/c1-5-17(23-3)15-25-19(21)13-11-9-7-8-10-12-14-20(22)26-16-18(6
InchiKey: BBVBWBRDMYGPAP-UHFFFAOYSA-N
Formula: C20H38O6
SMILES: CCC(COC(=O)CCCCCCCCC(=O)OCC(CC)OC)OC
Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-565.20	kJ/mol	Joback Method
hf	-1220.73	kJ/mol	Joback Method
hfus	48.46	kJ/mol	Joback Method
hvap	82.47	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.044		Crippen Method
mcvol	319.280	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	2151.00		NIST Webbook
tb	853.54	K	Joback Method
tc	1045.67	K	Joback Method
tf	473.94	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.21	J/mol×K	853.54	Joback Method
cpg	1109.52	J/mol×K	1013.65	Joback Method
cpg	1096.81	J/mol×K	981.62	Joback Method
cpg	1082.82	J/mol×K	949.60	Joback Method
cpg	1067.56	J/mol×K	917.58	Joback Method
cpg	1051.02	J/mol×K	885.56	Joback Method
cpg	1120.96	J/mol×K	1045.67	Joback Method
dvisc	0.0000248	Pa×s	853.54	Joback Method
dvisc	0.0000337	Pa×s	790.27	Joback Method

dvisc	0.0000482	Pa×s	727.01	Joback Method
dvisc	0.0000738	Pa×s	663.74	Joback Method
dvisc	0.0001237	Pa×s	600.47	Joback Method
dvisc	0.0002339	Pa×s	537.21	Joback Method
dvisc	0.0005246	Pa×s	473.94	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=R542179&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