Sebacic acid, di(5-methoxy-3-methylpentyl) ester

Inchi: InChI=1S/C24H46O6/c1-21(13-17-27-3)15-19-29-23(25)11-9-7-5-6-8-10-12-24(26)30-20
InchiKey: OENXKTXOEBGLAN-UHFFFAOYSA-N
Formula: C24H46O6
SMILES: COCCC(C)CCOC(=O)CCCCCCCCC(=O)OCCC(C)CCOC
Mol. weight [g/mol]: 430.62

Physical Properties

Property code	Value	Unit	Source
gf	-531.52	kJ/mol	Joback Method
hf	-1303.29	kJ/mol	Joback Method
hfus	58.82	kJ/mol	Joback Method
hvap	91.37	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	5.319		Crippen Method
mcvol	375.640	ml/mol	McGowan Method
pc	841.13	kPa	Joback Method
rinpol	2940.00		NIST Webbook
rinpol	2940.00		NIST Webbook
tb	945.06	K	Joback Method
tc	1160.91	K	Joback Method
tf	519.02	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.05	J/mol×K	945.06	Joback Method
cpg	1359.97	J/mol×K	1124.93	Joback Method
cpg	1347.97	J/mol×K	1088.96	Joback Method
cpg	1334.19	J/mol×K	1052.98	Joback Method
cpg	1318.62	J/mol×K	1017.01	Joback Method
cpg	1301.24	J/mol×K	981.03	Joback Method
cpg	1370.19	J/mol×K	1160.91	Joback Method
dvisc	0.0000133	Pa×s	945.06	Joback Method

dvisc	0.0000181	Pa×s	874.05	Joback Method
dvisc	0.0000262	Pa×s	803.05	Joback Method
dvisc	0.0000406	Pa×s	732.04	Joback Method
dvisc	0.0000691	Pa×s	661.03	Joback Method
dvisc	0.0001337	Pa×s	590.03	Joback Method
dvisc	0.0003099	Pa×s	519.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355512&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