Sebacic acid, 2-methoxyethyl tridecyl ester

Inchi: InChI=1S/C26H50O5/c1-3-4-5-6-7-8-9-10-13-16-19-22-30-25(27)20-17-14-11-12-15-18-2
InchiKey: MCLNTLKPWANDQA-UHFFFAOYSA-N
Formula: C26H50O5
SMILES: CCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCOC
Mol. weight [g/mol]: 442.67

Physical Properties

Property code	Value	Unit	Source
gf	-404.80	kJ/mol	Joback Method
hf	-1201.79	kJ/mol	Joback Method
hfus	69.86	kJ/mol	Joback Method
hvap	94.19	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	7.151		Crippen Method
mcvol	397.950	ml/mol	McGowan Method
pc	755.15	kPa	Joback Method
rinpol	3108.00		NIST Webbook
rinpol	3108.00		NIST Webbook
tb	969.28	K	Joback Method
tc	1198.00	K	Joback Method
tf	549.33	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1377.16	J/mol×K	969.28	Joback Method
cpg	1398.15	J/mol×K	1007.40	Joback Method
cpg	1417.20	J/mol×K	1045.52	Joback Method
cpg	1434.34	J/mol×K	1083.64	Joback Method
cpg	1449.61	J/mol×K	1121.76	Joback Method
cpg	1463.04	J/mol×K	1159.88	Joback Method
cpg	1474.68	J/mol×K	1198.00	Joback Method
dvisc	0.0002751	Pa×s	549.33	Joback Method

dvisc	0.0001307	Pa×s	619.32	Joback Method
dvisc	0.0000722	Pa×s	689.31	Joback Method
dvisc	0.0000445	Pa×s	759.31	Joback Method
dvisc	0.0000298	Pa×s	829.30	Joback Method
dvisc	0.0000212	Pa×s	899.29	Joback Method
dvisc	0.0000159	Pa×s	969.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355765&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

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