Sebacic acid, 2-methoxyethyl pentadecyl ester

Inchi: InChI=1S/C28H54O5/c1-3-4-5-6-7-8-9-10-11-12-15-18-21-24-32-27(29)22-19-16-13-14-1
InchiKey: QMFGRPDSAAVQQH-UHFFFAOYSA-N
Formula: C28H54O5
SMILES: CCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCOC
Mol. weight [g/mol]: 470.73

Physical Properties

Property code	Value	Unit	Source
gf	-387.96	kJ/mol	Joback Method
hf	-1243.07	kJ/mol	Joback Method
hfus	75.04	kJ/mol	Joback Method
hvap	98.64	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	7.931		Crippen Method
mcvol	426.130	ml/mol	McGowan Method
pc	681.36	kPa	Joback Method
rinpol	3309.00		NIST Webbook
rinpol	3309.00		NIST Webbook
tb	1015.04	K	Joback Method
tc	1267.21	K	Joback Method
tf	571.87	K	Joback Method
vc	1.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1505.96	J/mol×K	1015.04	Joback Method
cpg	1528.16	J/mol×K	1057.07	Joback Method
cpg	1547.93	J/mol×K	1099.10	Joback Method
cpg	1565.34	J/mol×K	1141.12	Joback Method
cpg	1580.45	J/mol×K	1183.15	Joback Method
cpg	1593.32	J/mol×K	1225.18	Joback Method
cpg	1604.01	J/mol×K	1267.21	Joback Method
dvisc	0.0002107	Pa×s	571.87	Joback Method

dvisc	0.0000984	Pa×s	645.73	Joback Method
dvisc	0.0000537	Pa×s	719.59	Joback Method
dvisc	0.0000329	Pa×s	793.45	Joback Method
dvisc	0.0000218	Pa×s	867.32	Joback Method
dvisc	0.0000155	Pa×s	941.18	Joback Method
dvisc	0.0000115	Pa×s	1015.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355767&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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